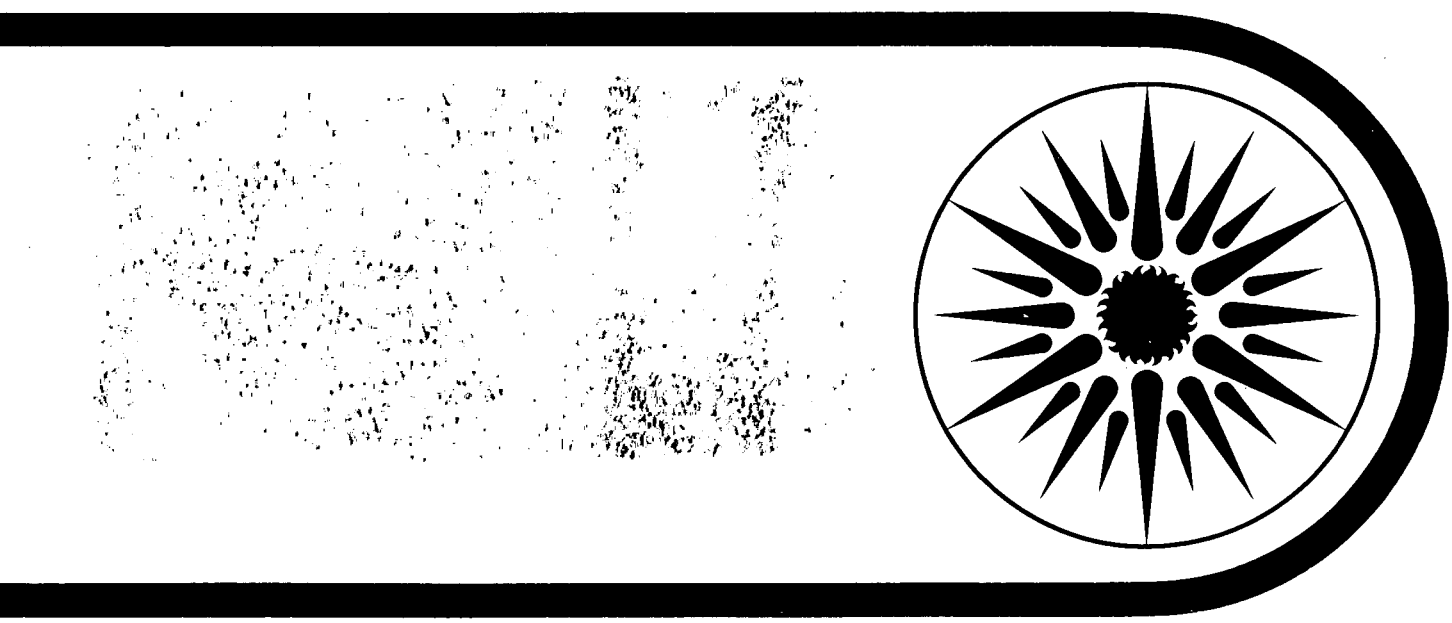
Annual Report

FY 1987

Applied Science Division

March 1988



Lawrence Berkeley Laboratory
University of California

Prepared for the U.S. Department of Energy under Contract DE-AC03-76SF00098

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LBL-24210

APPLIED SCIENCE DIVISION ANNUAL REPORT FY 1987

Elton J. Cairns

Head, Applied Science Division
and
Associate Director, LBL

Applied Science Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

Prepared for the U.S. Department of Energy under Contract No. DE-AC03-76SF00098

STATEMENT OF THE DIVISION HEAD

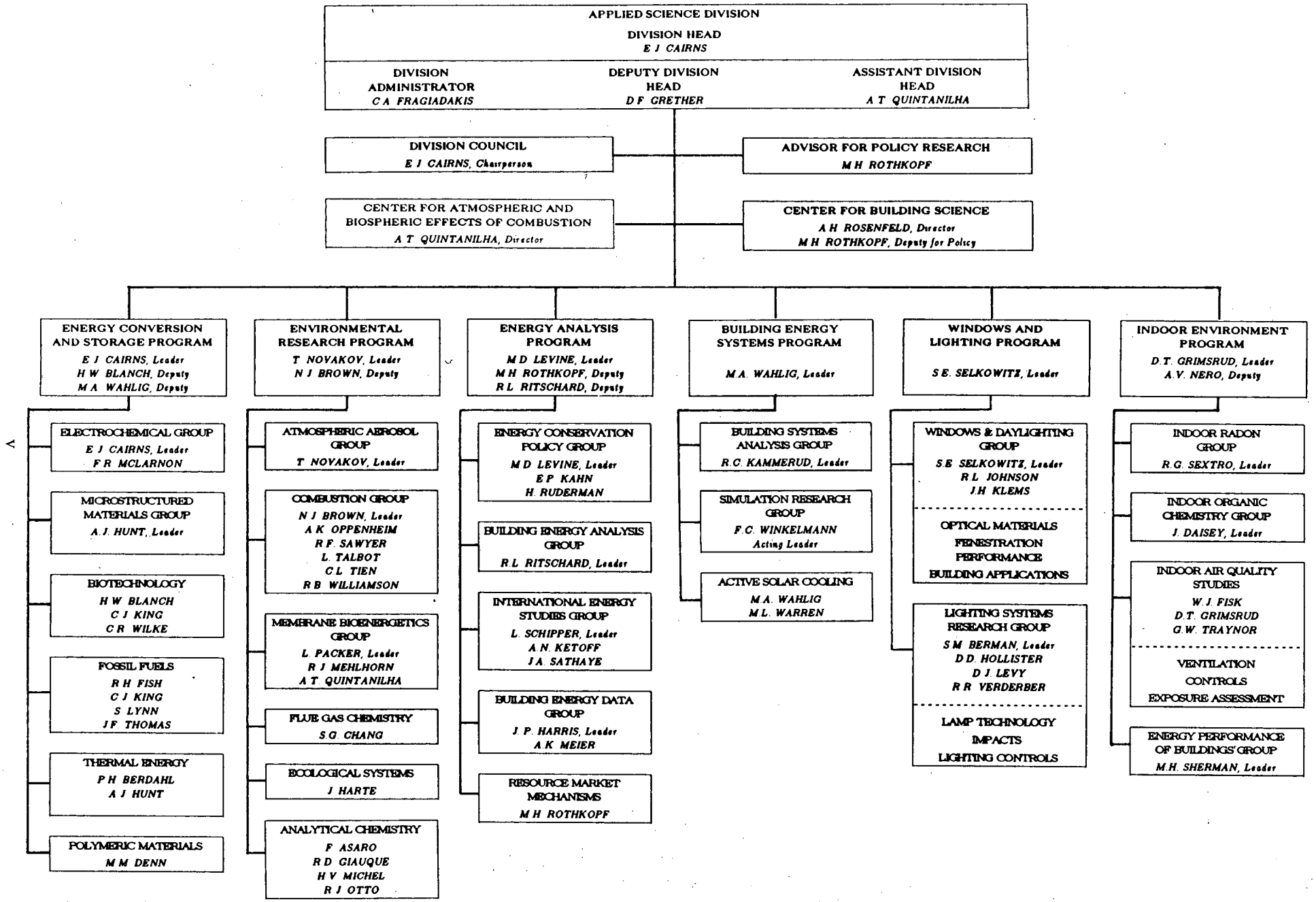
The Applied Science Division (ASD) of Lawrence Berkeley Laboratory (LBL) had its origins in the national concerns over energy and the environment in the early 1970's. The nation's attention to these issues has waxed and waned over the years; for example, the recent decline in the price of oil has led to a diminished interest in energy conservation. However, there is no doubt that over the longer term the nation must make more efficient use of energy and develop new energy sources, especially because oil imports are a large fraction of the growing trade deficit. Concerns over the health, environmental, and global climate impacts of energy use are increasing. The nation's international industrial competitiveness, for example for energy-related products, is an ongoing issue. The Division views its role as being in the forefront of the research effort that will help the nation address these concerns.

In 1987 the Division continued work in its major research areas: Energy Conversion and Storage (advanced batteries and fuel cells, solar and fossil fuel conversion, biotechnology, materials for energy applications), Environmental Research (atmospheric and biospheric effects of combustion, combustion processes, analytical chemistry, membrane bioenergetics), Building Sciences (advanced electrical lighting, windows, daylighting, and thermally driven heat pumps; building energy use measurement, computer simulation, and prediction; building data compilation and analysis; indoor air quality), and Policy Analysis (energy conservation relative to energy utilities, international energy demand, natural resource market mechanisms, appliance efficiency standards).

During 1987 the Division worked towards developing new and expanded research areas. In response to an opportunity provided by the Department of Energy (DOE), ASD took the lead in proposing a considerably enhanced indoor radon research program at LBL. ASD became the LBL participant in a joint DOE/Electrical Power Research Institute assessment of energy productivity applications of the newly discovered high temperature superconductors. Using Exploratory Research & Development funds, an environmental policy analysis activity was initiated. Progress was made in establishing a research program on energy efficiency that would be addressed to the needs of the State of California.

The Division had been reorganized in 1986: six new scientific Programs had been fashioned out of the former five Programs, and two Centers had been formed to coordinate research across Program boundaries: the Center for Building Science, and the Center for Atmospheric and Biospheric Effects of Combustion (CABEC). This new structure has turned out to serve the Division quite well, and in 1987 only a few changes to the organization proved necessary. The position of Director for CABEC was filled. The Indoor Environment Program was restructured somewhat to reflect personnel and programmatic changes. The *Summary of the Activities of the Applied Science Division* addresses the above subjects in more detail, describes the major research accomplishments for 1987, and provides other information concerning the Division. The individual Chapters provide more detailed descriptions of the work at the Group and Project level.

Elton J. Cairns
Associate Director and Division Head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E J CAIRNS
DIVISION ADMINISTRATOR
C A FRAGIADAKIS
DEPUTY DIVISION HEAD
D F GRETHER
ASSISTANT DIVISION HEAD
A T QUINTANILHA
DIVISION COUNCIL
E J CAIRNS, Chairperson
ADVISOR FOR POLICY RESEARCH
M H ROTHKOPF
CENTER FOR ATMOSPHERIC AND BIOSPHERIC EFFECTS OF COMBUSTION
A T QUINTANILHA, Director
CENTER FOR BUILDING SCIENCE
A H ROSENFELD, Director
M H ROTHKOPF, Deputy for Policy
ENERGY CONVERSION AND STORAGE PROGRAM
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M A WAHLIG, Deputy
ELECTROCHEMICAL GROUP
E J CAIRNS, Leader
F R MCLARNON
MICROSTRUCTURED MATERIALS GROUP
A J HUNT, Leader
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C J KING
C R WILKE
FOSSIL FUELS
R H FISH
C J KING
S LYNN
J F THOMAS
THERMAL ENERGY
P H BERDAHL
A J HUNT
POLYMERIC MATERIALS
M M DENN
ENVIRONMENTAL RESEARCH PROGRAM
T NOVAKOV, Leader
N J BROWN, Deputy
ATMOSPHERIC AEROSOL GROUP
T NOVAKOV, Leader
COMBUSTION GROUP
N J BROWN, Leader
A K OPPENHEIM
R F SAWYER
L TALBOT
C L TIEN
R B WILLIAMSON
MEMBRANE BIOENERGETICS GROUP
L PACKER, Leader
R J MEHLHORN
A T QUINTANILHA
FLUE GAS CHEMISTRY
S G CHANG
ECOLOGICAL SYSTEMS
J HARTE
ANALYTICAL CHEMISTRY
F ASARO
R D GIAUQUE
H V MICHEL
R J OTTO
ENERGY ANALYSIS PROGRAM
M D LEVINE, Leader
M H ROTHKOPF, Deputy
R L RITSCHARD, Deputy
ENERGY CONSERVATION POLICY GROUP
M D LEVINE, Leader
E P KAHN
H. RUDERMAN
BUILDING ENERGY ANALYSIS GROUP
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L. SCHIPPER, Leader
A N. KETOFF
J A. SATHAYE
BUILDING ENERGY DATA GROUP
J. P. HARRIS, Leader
A K MEIER
RESOURCE MARKET MECHANISMS
M H ROTHKOPF
BUILDING ENERGY SYSTEMS PROGRAM
M A. WAHLIG, Leader
BUILDING SYSTEMS ANALYSIS GROUP
R.C. KAMMERUD, Leader
SIMULATION RESEARCH GROUP
F.C. WINKELMANN
Acting Leader
ACTIVE SOLAR COOLING
M A. WAHLIG
M L. WARREN
WINDOWS AND LIGHTING PROGRAM
S E. SELKOWITZ, Leader
WINDOWS & DAYLIGHTING GROUP
S E SELKOWITZ, Leader
R L JOHNSON
J.H KLEMS
OPTICAL MATERIALS
FENESTRATION
PERFORMANCE
BUILDING APPLICATIONS
LIGHTING SYSTEMS RESEARCH GROUP
S M BERMAN, Leader
D D. HOLLISTER
D J. LEVY
R R VERDERBER
LAMP TECHNOLOGY
IMPACTS
LIGHTING CONTROLS
INDOOR ENVIRONMENT PROGRAM
D.T. GRIMSRUD, Leader
A.V. NERO, Deputy
INDOOR RADON GROUP
R.G. SEXTRO, Leader
INDOOR ORGANIC CHEMISTRY GROUP
J. DAISEY, Leader
INDOOR AIR QUALITY STUDIES
W.J. FISK
D.T. GRIMSRUD
G.W. TRAYNOR
VENTILATION
CONTROLS
EXPOSURE ASSESSMENT
ENERGY PERFORMANCE OF BUILDINGS GROUP
M.H. SHERMAN, Leader

APPLIED SCIENCE DIVISION

Elton J. Cairns

Division Head

Cheryl Fragiadakis	Donald F. Grether	Alex Quintanilha
Division Administrator	Deputy Division Head	Assistant Division Head

DIVISION OFFICE STAFF

Cynthia Bollinger	Helen Leung	Susan Petersen	Nancy Wishner
Eric Essman	Sandra Mocco	Rosa Rodriguez	Zenaida Yuson
Camelia Griego	Maria Ossa	Janet Smith	
Mary Hart	Rebecca Palmer	Angela Smothers	

ENERGY CONVERSION AND STORAGE PROGRAM STAFF

Elton Cairns, Program Leader
Harvey Blanch, Deputy Program Leader
Michael Wahlig, Deputy Program Leader

Thomas Adler
Daniel Arenson
Vincent Battaglia
Paul Berdahl
Ernest Blatchley
Garth Burns
Van Carey
Douglas Clark
Thomas Colson
Daniel Crean
Ayesha Daniels
Christian Daughton
Morton Denn
Gregory Dow
Katherine Dukes
Jean Dupon
Richard Fish
Raymond Fong
Alan Foss
Gad Friedman*
Antonio Garcia
Terry Grant
Edward Grens
Robert Guinn
Donald Hanson
Richard Hix
Isaac Hodara*
Paul Hsuin
Arlon Hunt
Mark Isaacson
Alejandro Izquierdo
Avieyer Kertes
Hoon-Sik Kim
C. Judson King
Kim Kinoshita
Judith Klinman
Gregg Langlois
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Laura Lindsay-Murphy
Kevin Lofftus
Scott Lynn
Frank McLarnon
Fletcher Miller
Kenneth Miller
Riley Moore
Stuart Naftel
Mindy Ng
Dan Neumann
Jon Noring
Loree Poole
Robert Price
William Rixey
James Rudnicki
Richard Russo
Richard Sakaji
Steve Sciamanna
Robert Selleck
Jon Spear
Charlotte Standish
John Starr
Craig Stevens
Kathryn Striebel
Janet Tamada
Jerome Thomas
Jeffrey Weaver
Charles Wilke

*Participating guest

ENVIRONMENTAL RESEARCH PROGRAM STAFF

Tihomir Novakov, Program Leader
Nancy Brown, Deputy Program Leader

Frank Asaro†
Henry Benner
Charles Blanchard
James Bonini
Nancy Brown†
John Cavolowsky
Shih-Ger Chang†
Robert Cheng
Peck Cho‡
Mariah Cochrane
John Dailey
Fernando Diaz*
Raymond Dod
Cheryl Ehorn
Eric Essman
David Faris
Charles Fleischman
Erica Fono
Stephanie Frolich
Ian Fry
Robert Giauque
Gloria Gill
Iskander Gokalp*
Ralph Greif
Lara Gundel
Patti Hannah
Anthony Hansen
John Harte
Jean Hertzberg
Kenneth Hom
Ke-Yuan Hu*
Wei-Ming Huang
Gary Hubbard
Margaret Huflejt
Frank Hurlbut
Kristine Ing
Allene Johnson
Johanna Lang
Chung Lau‡
David Littlejohn
David Liu
Donald Lucas
John Maguire
Samuel Markowitz
Richard Martin
Andrew Maxson
Rolf Mehlhorn
Harvey Michaels
Helen Michel
Fred Mowrer
Amos Newton
Tihomir Novakov†
Antoni Oppenheim
Roland Otto
Lester Packer†
Isadore Perlman
Ahmed Rashed
Wanda Reyes*
Chang Woo Rhee
Frank Robben
Eva Robinson
Douglas Rotman
Robert Sawyer
Frank Schipperijn
Richard Schmidt
Richard Schneider
Ian Shepherd§
Pauline Sherman
Linda Sindelar
Nicole Somorjai
Horton Stewart§
Fred Stross*
Lawrence Talbot
Su Weil-Han*
Eric Wakahiro
R. Brady Williamson
Linda Wroth

*Participating guest
†Group Leader
‡University of California Davis
§University of California Berkeley

ENERGY ANALYSIS PROGRAM STAFF

Mark Levine, Program Leader
Ronald Ritschard, Deputy Program Leader
Michael Rothkopf, Deputy Program Leader

Hashem Akbari
Anibal de Almeida*
Barbara Atkinson
Barry Barnes
Sarita Bartlett
John Beldock
Betty Bratton
John Brown
James Bull
John Busch
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Quinsan Cao
Kathleen Carlson
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Mark Christensen
Alan Comnes
Deborah Connell
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Philip Cunliffe
Diana DeBoer
Susan Ellis
Joseph Eto
Jean Ferrari
Anthony Fisher‡
Denise Flora
Sunita Gandhi
Rich Gilbert
Andre Ghirardi
Peter Goering
Charles Goldman
Kathleen Greely
Steven Greenberg
William Hanneman‡
Jeff Harris
Diane Hawk
Kristin Heinemeier*
Ali Heydari
Chean Yok Hsui
Yu Joe Huang
Ruri Immamura
Margaret Jackson
Adam Kahane*
Edward Kahn
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Margaret Knight
Jonathan Koomey
Florentin Krause
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Sharad Lele
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Jean-Michel Nataf
Bruce Nordman
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Samuel Oren‡
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Park Chun Hun*
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Christopher Pignone
Gaurev Prabhakar
Leo Raineir*
John Randolph
Imelda Reyes
Jacques Roturier*
Itzhak Ravid*
Henry Ruderman
Jayant Sathaye
Lee Schipper
Nancy Schorn
Renee Slonek
Timothy Springer
Steve Stoft
Haider Taha
Mounira Taleb-Ibrahimi
Ann Thorpe
Isaac Turiel
Dorothy Turner
Stephen Tyler
Edward Vine
Francis Wenger*
Deborah Wilson
David Wood
Winifred Yen-Wood

*Participating guest
†University of California, Davis
‡Affiliated staff

BUILDING ENERGY SYSTEMS PROGRAM STAFF

Michael A. Wahlig, Program Leader

Brandt Andersson
Bruce Birdsall
Fred Buhl
William Carroll
Dominique Dumortier
Kathleen Ellington
Ahmet Erdem
Barbara Erwine
Brenda Hatfield
Robert Hitchcock
Deborah Hopkins
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Benoit Lebot
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Jean-Michel Nataf
Ori Nour-Omid
Cindy Polansky
Joseph Rasson†
Edward Sowell‡
Charlotte Standish
Mashuri Warren
Kevin Whitley
Frederick Winkelmann*

*Group Leader
†Engineering Division
‡Participating guest

WINDOWS AND LIGHTING PROGRAM STAFF

Stephen Selkowitz, Program Leader

Dariush Arasteh
Erica Atkin
Charles Benton
Samuel Berman*
Robert Clear
Douglas Crawford
Dennis DiBartolomeo
Ellen Gailing
John Hartman
Mary Lou Hinman
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Jong Jin Kim
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Robert Richardson†
Michael Rubin
Francis Rubinstein
Michael Siminovitch
Stephen Selkowitz*
Jonathan Spear
Robert Sullivan
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Liang-Zhong Wang†
Gregory Ward
Richard Whiteman§
Michael Wilde
Ruth Williams
John Wolfe
David Wruck
Mehrangiz Yazdanian
Phillip Yu
Tai-Ming Zhou†

*Group Leader
†Participating Guest
‡Plant Engineering
§Engineering Division

INDOOR ENVIRONMENT PROGRAM STAFF

David Grimsrud, Program Leader
Anthony Nero, Deputy Program Leader

Janet Aceti
Kathleen Alevantis
James Allen
Michael Apte
Stephen Brown
Greg Chittick
Peter Cleary
Joan Daisey
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Theresa Lessard-Smith
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Gail Schiller
Richard Sextro†
Max Sherman†
Brian Smith
Bruce Springsteen
Harvey Sokol‡
Carol Stoker
Richard Szydlowski
Greg Traynor
Bradley Turk
Henrik Wallman

*Biology & Medicine Division
†Group Leader
‡Materials & Chemical Sciences Division

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APPLIED SCIENCE DIVISION

SUMMARY OF ACTIVITIES
FY 1987

I. INTRODUCTION

Fiscal Year 1987 (FY87) was a year of accomplishments and changes for the Division. Recent scientific accomplishments are summarized in Section II; trends in the research program of the Division are covered in Section III. The FY86 *Summary* described a number of past accomplishment of the Division which have had a significant impact on the larger society. This year, several additional accomplishments were judged to have had such an impact—they are described in Section IV.

Section V discusses organizational aspects of the Division. The final Section, VI, covers other activities and notable events.

II. RECENT SCIENTIFIC ACCOMPLISHMENTS

Summarized here are some of the recent accomplishments of the Division. These and other accomplishments are reported in more detail in the subsequent Chapters of the Annual Report. For purposes of convenience, this section is organized in the same manner as the Chapters, i.e, by the scientific Programs of the Division. Within a Program, the accomplishments are presented in no particular order.

Selected accomplishments are described in enough detail for the reader to gain something of the flavor of the background to, the nature of, and the significance* of the accomplishment. Briefer descriptions are provided of other accomplishments. For purposes of simplicity, only the name of the Principal Investigator(s) is given, although several other researchers will normally have been involved with any given accomplishment.

A. Energy Conversion and Storage Program

Application of Photothermal Deflection Spectroscopy to Identify Species in Electrochemical Cells (Elton Cairns)

The formation and disappearance of chemical species on an electrode surface and at the electrode-electrolyte interface plays a critical role in the performance and lifetime of electrochemical systems. Numerous spectroscopic, optical and surface-science techniques have been employed to characterize electrochemical systems, but their use is restricted by (i) the need for an ultra-high-vacuum environment, (ii) stringent electrode surface requirements, (iii) narrow regions of the optical spectrum, and/or (iv) specific chemical species. These restrictions have precluded the quantitative study of many important electrochemical systems, especially those that employ porous electrodes and multi-component electrolytes (e.g., batteries and fuel cells).

Photothermal deflection spectroscopy (PDS) is an ultrasensitive technique that can provide in situ measurement of chemical species at a solid surface or in an adjacent fluid. The ASD Electrochemical Group has adapted the PDS technique to study electrode surfaces and electrolytes of electrochemical cells. Recent experiments have demonstrated the ability of PDS to

*The significance of the accomplishment may be that it leads to an application, resolves a scientific issue, sets the stage for major new research directions, has the potential for making an impact on the larger society, and the like.

identify surface species in situ with extremely high sensitivity (to less than one monolayer of coverage of the bare electrode surface), to operate over a wide range of wavelengths, and to identify species in the electrolyte. In addition, PDS requires no special electrode preparation methods and is relatively insensitive to impurities.

The ASD Electrochemical Group will apply PDS to characterize batteries, fuel cells and other electrochemical technologies. The resulting unique information will lead to improved performance and lifetime of these technologies, and thereby increase their use in energy conversion and storage applications.

Other Recent Accomplishments of the Energy Conversion & Storage Program

- Developed microelectrodes to measure in situ species concentrations in rechargeable alkaline zinc cells. (Elton Cairns)
- Developed a comprehensive mathematical model of the rechargeable zinc/nickel oxide cell. (Elton Cairns)
- Demonstrated that polymer-electrolyte fuel cells can be constructed using electrodes containing one-tenth as much platinum as that in previous cells, yet exhibit comparable performance. (Los Alamos National Laboratory under LBL programmatic direction)
- Developed a rechargeable, high-temperature lithium alloy/molten-salt/iron disulfide cell with very high performance and long cycle life. (Argonne National Laboratory under LBL programmatic direction)
- Identified and analyzed factors governing the equilibria for extraction of carboxylic acids from aqueous solution by means of solvent systems composed of tertiary amine extractants in various diluents. This insight leads to several potential ways of reducing costs for recovery of carboxylic acids made from biomass by fermentation. These include more efficient regeneration of extractant by temperature swing and/or change of diluent composition. (Judson King)
- Shown that incomplete regeneration of phenols adsorbed on activated carbon results from an irreversible multimolecular reaction. Methods of regeneration and/or pretreatment of carbons to minimize this effect are being pursued. This research will serve to reduce costs of regenerated adsorption processes for removing phenols from effluent waters, such as condensate waters from low-temperature coal gasification. (Judson King)
- Examined the use of supercritical CO_2 as a solvent for enzyme-catalyzed reactions. Patent pending. (Harvey Blanch)

B. Environmental Research Program

Recent Accomplishments of the Environmental Research Program

- Developed an NMR method to follow the energy status of environmentally stressed cyanobacteria [blue-green algae]. Allows one to demonstrate the responses inside cells of their energy status when subjected to a sudden environmental stress, and the changes in energy status accompanying recovery from stress. Makes possible on a quantitative basis in intact cells a determination of the degree to which the environment will affect cell energy status. Can tell whether cells retain the capacity to survive a degree of stress. (Les Packer)
- Developed methods using thin-section electron microscopy [in collaboration with colleagues M. Lefort-Tran, M. Pouphille, and S. Spath] to show that the striking response of cyanobacteria to stress is massive accumulation of glycogen (carbohydrate) in the form of granules that are preferentially organized in the space between the cytoplasmic (plasma) membrane and internal membranes (involved in photosynthesis) of cyanobacteria [blue-green algae]. This finding is to be exploited for changing cell composition in order to utilize cyanobacteria [blue-green algae] as a food supplement for long-term manned planetary stations as part of the NASA CELSS program [closed ecological life support systems]. (Les Packer)

C. Energy Analysis Program

Recent Accomplishments of the Energy Analysis Program

- Completed final version of PEAR (Program for Energy Analysis of Residences) and released it to the public. (Ron Ritschard)
- Completed draft version of Utility Accounting System for use by local public housing authorities through a joint DOE-HUD project. (Ron Ritschard)
- Contributed to the *Energy-efficient Building Foundation Design Handbook* developed jointly with the Underground Space Center at the University of Minnesota. (Ron Ritschard)
- Demonstrated that the theoretical economic efficiency advantages of nondiscriminatory sealed bidding over standard sealed budding cannot be realized and would be small if achieved. (Mike Rothkopf)

E. Windows and Lighting Program

Electrochromic Optical Switching Devices for Windows (Carl Lampert)

Electrochromic optical switching devices have the potential to dynamically control transmittance as a function of climatic conditions and building energy requirements. The use of these films can reduce building energy consumption and increase productivity in the workplace. Other applications for this technology include glazings for automobiles, aircraft and spacecraft. Electrochromic devices can reversibly color and bleach by the application of a small voltage (1-3V). The device only uses power when a change in optical density is required. The films give high optical clarity over a wide range of optical densities.

In the Windows and Daylighting group, we are studying the properties of electrochromic hydrated nickel oxide. This compound switches from transparent to brownish-bronze color. This relatively new material has been developed at LBL. This material has cost and ease of fabrication advantages over other electrochromic compounds. To make an operational device, we have developed the device structure: glass/tin oxide/hydrated nickel oxide/polymer electrolyte/tin oxide/glass. In our continuing studies, we are characterizing and optimizing this device structure.

Design and Testing of a Highly Insulating Glazing System for Use with Conventional Window Systems (Dariush Arasteh, Stephen Selkowitz)

Conventional double-glazed windows (R2) are being replaced by double-glazed units with low-emissivity coatings and an argon gas-fill (R4). Higher-R windows (R6-10) offer added potentials; greater energy savings, design freedom to use more and larger windows on off-south orientations, increased occupant comfort, and reduced condensation.

The Windows and Daylighting Group has developed and tested a prototype design for an R8-R10 window. This design makes use of commercially available low-emissivity coatings, gases, and glazing materials. The unit being developed will fit in standard frame and sash designs and will not require extensive retooling on the part of window manufacturers. Tests in a laboratory hot-plate facility and the Windows and Daylighting Groups' Mobile Window Thermal Test Facility have validated center-of-glass calculations of the window's performance. An analysis of prototypes' structural performance using a finite-element code indicates roughly the same low breakage probability as double glazed units. Current work is aimed at producing commercial prototypes for use and testing in demonstration houses. Work on specific issues (i.e., reducing frame and edge heat transfer, improving gas filling techniques, etc.) also continues.

F. Indoor Environment Program

Macromodel to Assess Indoor Air Pollution Concentration Distributions in U.S. Residences (Gregory Traynor)

The distribution of indoor air pollution levels in residences is not well known because the number of measurements is very low compared with the number of residences in the U.S. A novel approach to modeling the distributions of indoor air pollution concentration distributions has been developed at LBL for describing the indoor concentration distributions of carbon monoxide, nitrogen dioxide, and respirable suspended particles in single family residences. Ongoing and future research will be directed at generalizing and expanding the macromodel to include other pollutants (e.g., radon and organic pollutants) and multifamily residences. This new approach to modeling indoor air pollutant concentrations will allow policy makers, health officials, and others to identify high risk populations and will provide information needed to conduct risk assessments and epidemiology studies of indoor air pollution.

Residential Exhaust Ventilation With Heat Recovery (William Fisk)

In a relatively new method of mechanically ventilating residences, an exhaust fan draws air (typically from kitchens and bathrooms), directs this air through a small heat pump, and then exhausts the air to outside. Outdoor air is thus drawn into the residence through cracks and slot ventilators (essentially adjustable-size openings) in exterior walls. The heat pump, called an exhaust-air heat pump, extracts (recovers) heat from the exhaust airstream and transfers this heat to the hot water and/or the indoor air, thus reducing the normal water and space heating loads. A fairly comprehensive preliminary evaluation of this ventilation technology was completed in 1987. Through computer modeling, we determined that ventilation rates can be very stable in an exhaust-ventilated residence, that yearly energy savings in all-electric Pacific Northwest residences should typically range between 6000 and 8000 kWh, and that the cost of saving this energy would be approximately 3.5 to 4.6 cents per kWh which is similar to current electricity prices. Through other computer modeling, we estimated the impact of exhaust ventilation on radon entry rates and indoor radon concentrations. This modeling indicated the types of housing and soil conditions for which exhaust ventilation is likely to significantly aggravate (or in some situations reduce) indoor radon problems. Laboratory monitoring of exhaust-air heat pump thermodynamic performance was also completed. The measured data allowed us to verify and improve initial predictions of energy savings and also helped to identify an improved heat-pump control strategy which could lead to roughly 1000 kWh of increased energy savings per year.

Radon Control Methods (Brad Turk)

Investigations of methods to reduce indoor radon concentrations in homes with elevated levels have been conducted in two regions of the country—the Pacific Northwest and north-central New Jersey. Several different mitigation systems have been examined; in some cases more than one system was installed in each house so that a side-by-side comparison of their individual effectiveness could be made. Indoor radon levels were reduced in each house in which the experiments were conducted. In some cases, the reductions were as large as 99%; in all cases, the average concentrations in the basement were less than the EPA guideline of 4 pCi/L.

These two regions have a number of important differences regarding both soils and typical house construction features; these characteristics in turn meant that there were significant differences in the installation and operational details of the control systems. One such difference was the air permeability and the radon content of the soil in the two regions. In the Pacific Northwest, certain mitigation measures, such as subslab pressurization were effective, probably due to the high permeabilities and relatively low radon in soil gas. In contrast, the

soils in the vicinity of the study homes in New Jersey were generally less permeable and had higher soil gas radon concentrations. In these areas, subslab pressurization was not very effective as a control technique.

These experiments have helped demonstrate both the feasibility and practicality of radon control techniques designed to prevent or limit radon entry into houses. In addition, preliminary diagnostic techniques have been developed to assist in selecting and operating mitigation systems. Currently, follow-up evaluations of the mitigation systems that have been installed are underway in order to examine their durability and long-term effectiveness.

Other Recent Accomplishments of the Indoor Environment Program

- Developed and field-tested a model linking residential space heating requirements to indoor air pollution concentrations due to space heating sources. (Gregory Traynor)
- Identified semivolatile and nonvolatile organic contaminants as important pollutant groups emitted from unvented kerosene heaters. (Gregory Traynor)
- Modeled the influence of natural infiltration, balanced mechanical ventilation, and mechanical exhaust ventilation on radon entry rates and indoor radon concentrations. (William Fisk)
- Used multiple tracer gases to monitor ventilation rates, ages of air, airflow patterns, and ventilation efficiencies in commercial buildings. (William Fisk)
- Produced a preliminary map of and obtained distributional statistics for near-surface radium concentrations for the U.S. to investigate their use as partial indicators of regional radon potential. (Ken Revzan)
- Developed a parametric model for radon entry into houses, based on fundamental physical factors describing soil gas entry and radon removal by natural ventilation. This model was used to examine continuous radon data obtained during a year-long study conducted in seven New Jersey homes (Ken Revzan).
- Examined the integrating properties of charcoal-based passive radon monitors used for short-term measurements of radon concentrations indoors. The theoretical and experimental results were in good agreement, and generally showed that such charcoal-based monitors did not respond well to fluctuating levels often seen in homes with elevated radon levels, although the response characteristics were dependent upon the design of the device. (Rich Sextro)
- Verified experimentally that toxic volatile organic compounds from hazardous waste sites can enter buildings by pressure-driven flow of contaminated soil gas. (Joan Daisey)
- Measured and modeled indoor exposures to methylene chloride from the use of paint removers in residences and identified strategies to reduce exposures. (Joan Daisey)
- Evaluated the efficiency of selected portable air cleaners for removing NO_2 and volatile organic compounds and found that several have potential usefulness for this application. (Joan Daisey)
- Found that emissions of volatile organic compounds from materials used to finish interiors of large office buildings can be of the order of kilograms per day and may approach limits set by regulatory agencies for ozone control. (Joan Daisey)
- Demonstrated that concentrations of total volatile organics in a large, new office building were in the range shown to have irritant effects in sensitive individuals. (Joan Daisey)
- Found in a pilot study that woodburning stoves increased the indoor concentrations of polycyclic aromatic compounds, some of which are carcinogens, 2- to 46-fold. (Joan Daisey)

III. RESEARCH TRENDS

The New High-Temperature Superconductors

During FY 1987, the technical, semitechnical, and popular literature was filled with articles about the recently discovered high-temperature ceramic superconductors. At LBL, the bulk of the research is being carried out by the Materials and Chemical Sciences Research Division (MCSD). However, there is an emerging role for the Applied Science Division in assessments of potential applications of the new superconductors and, possibly, in the materials area as well.

ASD is the LBL participant in an assessment of applications that would conserve energy or (more broadly) improve energy productivity. The study is being jointly conducted by DOE/Conservation and the Electric Power Research Institute (EPRI). The overall study includes motors, magnetic separation processes, transportation, lighting, magnetic heat pumps, and electromagnetic pumping. [DOE/CRE has conducted a separate assessment of applications for generation, distribution, and storage of electricity.] LBL's principal areas of involvement are in assessing the potential applications for electric lighting (Sam Berman), and in establishing the basic processes and examining novel concepts (Paul Berdahl). The assessments were underway in late FY87 and will extend on into FY88.

Several ASD researchers have expertise and facilities that are potentially applicable to producing and investigating the new superconductors. Mike Rubin of the Windows & Daylighting Group has developed a sputtering system which is being used to investigate new types of thin-film coatings for windows. The same equipment and similar techniques are thought to be capable of producing a superconducting thin film. Rick Russo of the Energy Conversion & Storage Program is developing laser ablation as a way of characterizing the surface properties of materials. Similar methods at other institutions have been used to produce thin-film superconductors from abalated material. Finally, Arlon Hunt of Energy Conversion & Storage has been working for some time on the sol-gel process for fabricating ceramics for various applications. The process may well be applicable for making both bulk and thin-film superconductors. During FY 1988 the Division will be looking for opportunities to pursue these various approaches.

Environmental Policy Research

The Applied Science Division traces its origins back to an Environmental Program that was started at LBL around 1970. The early research, which continues today in the Environmental Research Program, focused on laboratory and field work in which sophisticated instruments and techniques were applied to environmental problems. Another early effort of the Division had to do with environmental assessments carried out by the Energy Analysis Program. Topics included: the estuarine impacts of fossil-fuel based technologies, the groundwater impacts of enhanced oil recovery, and growth and energy development in the rural west. These types of environmental studies came to an abrupt end in 1981.

Recently, there has been increasing concern over the impact that our technological society is having (or will have in the future) on the environment. Areas that have received media attention include: the warming of the atmosphere from CO_2 build-up; the hole in the ozone layer that may be caused by freon and other chlorofluorocarbons; and the European forests that are dying, perhaps from acid rain. Almost all of these are related in one way or another to energy. CO_2 and acid rain result from the combustion of fossil fuels. Freon is used extensively in refrigeration systems.

The Division is responding to this heightened interest in environmental issues. The Division's Center for Atmospheric and Biospheric Effects of Combustion is one such response (see Section V). Another is the new (or perhaps reborn) Environmental Policy Research effort within the Energy Analysis Program. This effort was started in FY87 by Mark Levine, Ron Ritschard, and others with internal Laboratory funding (Program Development Funds). These investigators have developed ties with UC researchers from several campuses, and have had

preliminary discussions with potential sources of funding. Out of these discussions emerged a number of key policy issues which are candidates for initial assessments, such as environmental risk assessment, environmental toxicology: indoor and outdoor pollutants, ecosystem effects of global climate change, and cost/benefit analyses of environmental regulations.

In addition, a national search was conducted for a high-caliber scientist to lead the activity. The search resulted in the hiring of two scientists with quite different but complementary skills who will start at LBL in early FY88. Walter Westman was most recently a National Research Council Resident Research Associate, Office of Ecosystem Science and Technology, at NASA/Ames Research Center; and formerly a Professor of Environmental Studies in the Department of Geography at UCLA (1976-1984). Paolo Ricci was a senior project manager at EPRI in the area of risk-benefit assessment, a senior scientist at Arthur D. Little in the area of health risk and benefit assessments, and most recently developed a risk assessment program for Italy.

Indoor Radon Research

As a result of the work at LBL and elsewhere, radon has recently received national attention as a health risk in single-family residences. In response, the DOE Office of Health and Environmental Research (OHER) has been increasing its support for radon-related research. In FY87, the Division received a significant funding increase for its ongoing radon characterization research, which includes work on soil transport, entry mechanisms, and indoor levels of radon. In addition, the Biology & Medicine Division received support for a new project on cell transformation by radon decay products.

In early FY87, OHER solicited peer-reviewable proposals from the National Labs, universities, and other institutions in anticipation of a yet larger radon research program in FY88. ASD's Anthony Nero organized a series of internal LBL seminars and a workshop with national attendance. A position paper was prepared, giving LBL's view of a comprehensive national research program, and congressional testimony was given by Donald Grether on the need for such a program.

Out of these activities, eight proposals to OHER were developed among four Divisions: Applied Science, Biology & Medicine, Earth Sciences, and Information & Computing Sciences. The proposed research includes: an epidemiological study of lung cancer mortality and indoor radon; surface spectroscopic studies of the mechanism of radon, precursor (uranium), and daughter (lead) attachment to geologic substrates; a comparison of radon availability and migration through various soils by means of small instrumented structures and controlled leakage characteristics; mathematical modeling of radon migration through soils and into buildings; indoor atmospheric chemistry—interactions of radon with other gaseous pollutants; interactions of radon and radon progeny with environmental tobacco smoke; and the critical analysis and integration of radon research for exposure, dosimetry, and risk assessment.

At the end of FY87, OHER was still undertaking its review process and thus had not yet selected the proposals to be funded.

IV. THE IMPACT OF PAST ACCOMPLISHMENTS

During FY86, the Division took stock of its research accomplishments which have had (or had the clear potential of having) a significant impact on the larger society: the scientific community, industry, the marketplace, and/or government decision making. The impact is generally recent and/or ongoing, although the actual research may have taken place some time ago. The FY 1986 *Summary of the Activities* provided brief descriptions of 19 such accomplishments.

During 1987, several additional accomplishments were judged to have had a significant impact on society. They are presented here in no particular order. For simplicity, only the names of the Principal Investigators are given, although several other researchers will normally have been involved with any given accomplishment.

Multiple Thin Films For Both High Reflectivity and High Transmission for Luminaires and Lamps (Rudy Verderber)

Background: (a) Luminaires can be made more efficient by employing highly specular reflecting surfaces and increasing the transmission of visible light through lenses. (b) Highly efficacious incandescent lamps can be obtained by coating a properly shaped envelope with a selective reflecting film—one that transmits the visible but reflects the infra-red radiation back onto the filament.

LBL Role: (a) In 1980, LBL initiated a cost shared program with a thin-film coating company to examine the efficiency of luminaires that were coated with multiple coatings of dielectric films. The study showed that luminaires with the thin film coated surfaces were 30% more efficient than the same luminaire design made with standard materials. (b) In 1979, LBL studied the status of energy efficient lamps that could be used in place of the standard incandescent lamp. One of the technologies was an incandescent lamp coated with a thin film that could reflect the emitted infra-red radiation back onto the filament. LBL measurements showed that the efficacy of a standard 15 lumen/watt lamp could be doubled.

Significance: (a) Based upon the LBL report, a small distribution company, Omega Energy, set up manufacturing facilities to employ these multiple dielectric coatings on fluorescent luminaires. The company, OCLI, that did the study with LBL is coating the materials for Omega Energy. These films have attained reflectances comparable to the more common specular coated surfaces (silver) but the added significant benefit is their durability of maintaining their integrity compared to existing technologies. More than 500 million luminaires are in place, requiring an average of 140 watts each. They are operated about 3000 hours annually, consuming 200 billion kWh. If only half of these fixtures could be refitted to improve their efficiency, 20 percent of the savings in electricity could be 21 billion kWh annually. (b) The active role of DOE and LBL in the transfer of these technologies through specific research and reports encouraged further development of this technology. Today, Duro-Test Corporation is manufacturing these efficient coated incandescent lamps. General Electric also employs these type of coatings on their high-wattage lamps to increase their efficacy. These lamps could be used in 10 percent of the incandescent market that consume 20 billion kWh of energy, and could reduce the consumption by 5 billion kWh annually.

Distribution of the WINDOW Program (Dariush Arasteh, Mike Rubin)

Background: Transferring to industry the technology developed under Department of Energy sponsorship is both a necessity and a continuing challenge. While there are ongoing and relatively standard approaches to technology transfer (e.g., reports, licensing of patents) there is also a need for innovative approaches by both DOE-supported research institutions and industry.

LBL Role: The Windows and Daylighting Group has continuously been developing a solar and thermal heat-transfer model for windows. Originally this program was used only as an in-house tool for evaluating the performance of window systems. In July 1986, a PC-compatible version, WINDOW 2.0, was distributed to about 100 major manufacturers of window products. The program was favorably received partly because the procedure was well documented and backed by a national laboratory. The Windows Group, however, had neither the time nor resources to distribute and support the program among the remaining 2000 smaller window manufacturers.

Significance: In July 1987, one very large user with ties to the entire extended window industry (Bostik Construction Products Division of the Emhart Chemical Group) agreed to reproduce and distribute the diskette and manual. The program was presented as a professional courtesy by Bostik with credit properly given to LBL and DOE. Bostik used a three-level approach to the distribution: (1) direct mail, (2) direct distribution by Bostik sales force, and (3)

trade show distribution. By these methods, Bostik estimates that companies representing more than half of all insulating glass industry sales have been reached with over 500 program users.

Additional technical and user features are being incorporated in a new version of the program, WINDOW 3.0. WINDOW is being used by ASHRAE for data to be included in the 1989 Handbook of Fundamentals and incorporates recent LBL research for ASHRAE TC4.5 and the National Fenestration Council.

Pressure-driven Flow as a Source of Radon in Houses (W. Nazaroff, A. Nero)

Background: Early radon research focused on release and diffusion of radon from crustal materials or water as major sources of indoor radon. However, research at LBL and elsewhere showed that radon emanation from building materials or diffusive flow from soils were too small to account for observed levels. With the further discovery of indoor concentrations substantially above average, these sources could be eliminated unequivocally as contributing significantly to high indoor radon levels. At the same time, research on building dynamics and infiltration indicated that the lower levels of residential structures had small, but persistent negative pressures with respect to ambient pressures. Such pressure differences provide the driving force for air infiltration; similar pressure-driven flow of radon-bearing soil gas into buildings could also occur via openings in the substructure.

LBL Role: Following an assessment of data obtained from one midwestern house, along with observations reported in the literature, the role of pressure-driven flow of radon-bearing soil gas into homes was more evident. A series of experiments employing tracer gases injected into the soil and using a blower door to artificially depressurize two houses demonstrated that soil gas flow into houses can occur and that the volumes and flow rates are consistent with the observed radon concentrations indoors.

Significance: With the importance of convective flow of radon understood, the effects of house dynamics and building operation have become more apparent. Current studies of radon entry into homes have included measurements of these parameters. At the same time, the role of soil-air permeability was recognized. This, in turn, has led to further research, both in the U.S. and abroad, on soil characteristics and air flows through various soils at both the local (i.e., house scale) and regional levels. Finally, the effectiveness of radon mitigation techniques designed to eliminate or reduce radon gas flow into homes has been demonstrated. Since many of these techniques are based on the concept of eliminating or reversing the pressure difference across the building shell, understanding the concept of pressure-driven flow of radon into buildings has made a significant contribution to the design and operation of successful radon control strategies.

Another aspect of this work has been the recognition that other potentially important indoor pollutants may also enter houses via pressure-driven flow of soil gas. In particular, soils in the vicinity of municipal landfills or hazardous waste sites have been shown to be contaminated with volatile organic chemicals (VOC), which can be transported by convective flow through soils and into houses. Research on this potential source of VOC indoors is currently underway at LBL.

V. Organizational Activities of the Division

The FY86 *Summary of Activities* described the reorganization of the Division. Briefly, six scientific **Programs** of roughly equal size were formed from the previous five Programs, with like work and funding sources consolidated. **Centers** were introduced to coordinate multidisciplinary efforts across Program boundaries in a matrix-like approach. The **Group** was recognized as the basic working unit of the Division. The Principal Investigator (PI) policy was modified to provide entry into the system for promising junior scientists as **Co-PI's**.

Overall, these changes worked well. The Division has functioned better administratively and has constructively focused attention on personnel development and future directions. One aspect of the Division's organization received further attention. The Indoor Environment Pro-

gram had, as in interim measure, been set up with two Groups having acting Leaders, and an authority structure which was incompletely reflected in the formal organization of the Program. In order to have a more regular structure for the Program, an Indoor Air Quality Studies research area was established in place of the Groups with acting leaders, and Anthony Nero was appointed the Deputy Program Leader. In addition, Joan Daisey, a senior chemist, joined the Program as the Leader of the Indoor Organic Chemistry Group.

The Center for Building Science, with Arthur Rosenfeld as Director, continued to concentrate on establishing the California Institute for Energy Efficiency (CIEE). With encouragement from the California Energy Commission and the California Public Utilities Commission, CIEE would coordinate research at LBL, the campus of the University of California, and other California research institutions. Funding would be provided by the California energy utilities, and the technology would be transferred back to the utilities for the ultimate benefit of California rate payers. This and other activities of the Center are described in more detail in the *Overview of the Center for Building Science.*

The FY86 *Summary of Activities* described various setbacks to the Center for Atmospheric and Biospheric Effects of Combustion (CABEC). In FY87, Alex Quintanilha, who had been coordinating the activities of the Center, was appointed as Center Director. The Center became involved in efforts of the DOE/Office of Health and Environmental Research (OHER) to define a new research program in the area of global climate change. This and other activities of the Center are described in more detail in the *Overview of the Center for Atmospheric and Biospheric Effects of Combustion.*

VI. Other Activities and Notable Events

Craig Hollowell Lecture

Craig Hollowell was a Senior Scientist in the Division and, until his untimely death in January, 1982, the leader of our indoor air quality research program. In 1983, the Craig Hollowell Lecture Series on Energy and the Environment was established as a memorial to Craig and as a way of providing recognition to outstanding scientists in the energy and environment fields. The first four lecturers have set a high standard. They were:

Year	Lecturer	Institution	Lecture Subject
1983	Jan A. J. Stolwijk	Yale University	Indoor Air Pollution: Exposure and Health Effects
1984	Tihomir Novakov	LBL	Smoke, Soot, Fog in the Atmosphere– From London to Los Angeles and Back
1985	Peter Schwartz	Shell Group	What Happened to the Energy Crisis?: The Dilemma of an Energy Decision Maker in a Dynamic World
1986	Samuel Berman	LBL	Shedding a Little Biophysics on Light: A New Visual Photometry

The calendar year 1987 lecture will be given in November by Mary O. Amdur of the Massachusetts Institute of Technology on *Combustion-generated Acid Aerosols: An Interdisciplinary Bridge from Stack to Lung*

Awards, Honors, Other Recognition

Person	Award/Honor/Recognition
Les Packer	In Kiev, the Institute of Physiology awarded Packer the Palladin Medal.

Antoni Oppenheim	1987 Dionizy Smolenski Medal of the Polish Academy of Sciences "for outstanding contributions towards advances in the knowledge of combustion and especially to dynamics of explosions and reactive systems."
Rudy Verderber	Received the Romain W. Myers Memorial Award, presented by the Golden Gate Section of the IES.
Carl Lampert	Service Citation for furthering the goals of SPIE-The International Society for Optical Engineering.

Service to the Scientific Community

The following is a partial list of such service for FY87.

Person	Activity
Les Packer	Clark Kerr Campus, University of California, Berkeley: Organized Workshop on the Biomedical Implications of Oxygen Radical Species in Cancer Promotion, Cancer Prevention, and Cancer Therapy. Organized International Summer School on New Developments and Methods in Membrane Research and Biological Energy Transduction. Satellite Meeting of the Society for Free Radical Research. Reelected to the International Union of Biochemistry (IUB) Committee on Symposia. Reappointed to UNESCO Expert Committee on Biomaterials for the European region and North America. Editor, *Archives of Biochemistry and Biophysics*, 1966 to present. Executive editor, Biological Oxidation and Bioenergetics Section, 1973 to present. Executive editor, Microsomes, Cytochrome P_{450} and Oxidase Section, 1984 to present. Editor, *Journal of Ultrastructure Research*, 1986 to present. Editor, *Journal of Free Radicals in Biology and Medicine*, 1986 to present. Vice President and Treasurer, International Society of Myochemistry.
C. Judson King	Council for Chemical Research: Director (1986-89); Vice Chairman (1987-88); Chairman (1988-89). Director, American Institute of Chemical Engineers (1987-89). National Research Council: Chairman, Committee on Separation Science and Technology, Board on Chemical Sciences and Technology; report, "Separation and Purification: Critical Needs and Opportunities," published 9/87. Chairman, Panel for National Engineering Laboratory, Board on Assessments of National Bureau of Standards Programs. National Academy of Engineering: Chairman, Peer Committee for Chemical Engineering (1988).
Elton Cairns	USA National Secretary, International Society of Electrochemistry Vice President, The Electrochemical Society Divisional Editor, *Journal of the Electrochemical Society.* Regional Editor, *Electrochimica Acta.* American Institute of Chemical Engineers: Chairman, Energy Conversion Committee.

Kim Kinoshita	Divisional Editor, Energy Technology Division, *Journal of the Electrochemical Society.*
Frank McLarnon	Organized battery sessions for the Intersociety Energy Conversion Engineering Conferences.
Joan Daisey	Served as Secretary of the Board of Directors of the American Association for Aerosol Research. Served on the Peer Review of the Love Canal Full-Scale Sampling Plan. Appointed to the U.S. EPA Science Advisory Board Committee on Indoor Air Quality and Total Human Exposure. Appointed to the American Conference of Governmental Industrial Hygienists Committee on Air Sampling Procedures. Appointed to the National Research Council Committee on Advances in Assessing Human Exposures to Airborne Pollutants.
Rudy Verderber	Vice President, Golden Gate Section, Illuminating Engineering Society.
Carl Lampert	General Editor, *Solar Energy Materials* (International, refereed, archival research journal). Conference organizer and Chairman, Optical Materials Technology for Energy Efficiency and Solar Energy Conversion VI, August 18-19, 1987, San Diego, CA. Member of conference organizing committee, SPIE-The International Society for Optical Engineering Lead U.S. representative on the International Energy Task X, Solar Materials.
Ron Ritschard	Continued membership on ASHRAE 90.2P committee that completed in FY 1987 a draft standard for *Energy Efficient Design of New Low Rise Residential Buildings.*
Mike Rothkopf	Established a new section on Practice in the journal *Operations Research.*
Michael Wahlig	Organized joint U.S.-Israel Workshop on Absorption Technology: Progress and Problems, held in Washington, D.C., 23-24 April 1987.
Harvey Blanch	Chairman, Engineering Foundation Conference "Enzyme Engineering," Santa Barbara, California, October 1987. Chairman, BioChemE Tutorial Sessions, American Institute of Chemical Engineering Annual Meeting, New York, November 1987.

CENTER FOR ATMOSPHERIC AND BIOSPHERIC EFFECTS OF COMBUSTION

SUMMARY OF ACTIVITIES FY 1987

The Center for Atmospheric and Biospheric Effects of Combustion (CABEC) provides an umbrella for similarly interested groups in different programs within the Applied Science Division, other Lawrence Berkeley Laboratory divisions, and other University of California departments to 1) perform joint research; 2) develop new research areas; 3) share resources; and 4) publish together. A Director was appointed in January 1987, and several research themes meriting increased effort have been identified.

Recognizing that deposition of acids and oxidants leads to major atmospherically mediated perturbations of the biosphere and arises from combustion processes, and given the areas of expertise within the Applied Science Division, we intend to emphasize three major research goals: 1) to accurately distinguish between local and long-range sources in the processes of deposition; 2) to determine the synergistic effects of acids and oxidants on plants; and 3) to study the mechanisms of oxidant-mediated damage to animals. A major effort will be planned to effectively combine the areas of atmospheric/combustion chemistry and physics with fundamental studies in cellular/molecular biology, physiology, ecology, and medicine. As an integral component of this effort, new and sensitive techniques would be developed to measure atmospheric deposition as well as biological damage and adaptation.

Because oxidative stress to cells and tissues has become an important area of study in diverse fields (particularly forest ecology, mutagenesis and carcinogenesis, aging, toxicology, and immune deficiency) and because several well-known groups at LBL and in the Bay Area are investigating this subject, recent workshops on oxidative injury have attracted a large number of scientists. As a result of these meetings, several joint proposals were developed for submission to a variety of funding agencies. We expect work in this area to increase, attracting several additional researchers to the Division.

CENTER FOR BUILDING SCIENCE

SUMMARY OF ACTIVITIES
FY 1987

RATIONALE

The Center for Building Science must be viewed in the larger context of the continuing national need for research on the efficient use of energy in buildings.

Buildings are the major energy consumer in the United States. In 1984, the U.S. buildings sector used $170 billion worth of energy, mainly as electricity. Of total annual U.S. electricity sales of $150 billion, most ($110 billion) was used for operating building equipment, lighting, and appliances. Use of fuels in buildings is also substantial ($60 billion of $290 billion).

Since 1973, rising energy prices and awareness have reduced our energy bills remarkably. Although since 1973 our stock of households has grown by 25% and commercial floor space has increased by 32%, primary energy use in buildings increased only 11%. Thus, energy use per square foot has fallen by 13% and $22 billion per year less is being spent than would be if historical trends in energy use had continued.

Substantial energy savings can be realized by retrofitting existing buildings and by constructing efficient new buildings. One way to estimate these potential savings is to use a "least cost" scenario that maximizes life-cycle cost effectiveness. A recent study for the state of Michigan indicates that, by the end of a 20-year period of new construction and retrofitting, a least-cost approach would save about one-third of the usual energy cost.

Building-energy research accelerates the capture of such potential energy and cost savings by 1) developing innovative concepts that lead to energy-efficient products on the market (e.g., advanced electric lighting systems, advanced windows); 2) understanding the performance of actual buildings (e.g., energy-loss mechanisms); 3) predicting the performance of new approaches (e.g., daylighting); and 4) developing the tools (e.g., computer programs) for designing efficient buildings and for understanding the effect of building standards. In addition, research is critical for understanding the human health and productivity implications of buildings (e.g., indoor air pollution and the effect of lighting on human performance). Finally, analytic studies can help predict the impact of energy-related government policies and programs on consumers, on the building industry, and on the energy utilities.

STRUCTURE

The Center for Building Science provides a structure for groups in different programs but with similar interests to perform joint research, to develop new research areas, to share resources, and to produce joint publications. The Center plans future building-science research, obtains funding for research, transfers building science R&D results to industry, and serves as a point of contact for building-science work at Lawrence Berkeley Laboratory. The list of publications following this description illustrates one type of activity for achieving these goals.

About 140 people are involved in activities of the Center and work in four different programs: Energy Analysis, Building Energy Systems, Windows and Lighting, and Indoor Environment. The accomplishments of these programs are reported in the chapters of this annual report. Center activities for promoting energy efficiency and for obtaining research funds are described next.

CALIFORNIA INSTITUTE FOR ENERGY EFFICIENCY

In 1986, the Center Director and others from the Applied Science Division and the Universitywide Energy Research Group (UERG) conceptualized a research program on energy end-use and efficiency that would address the needs of California. An organizing committee was formed, and the concept was named the California Institute for Energy Efficiency (CIEE). The goals of this institute were:

1) to carry out a mid-term research program based primarily on the expertise of LBL and the UC campuses, but involving other California research and education institutions;
2) to receive financial support from California energy utilities (e.g., PG&E);
3) to receive institutional backing from the California Public Utilities Commission (CPUC) and the California Energy Commission (CEC);
4) to establish mechanisms for transferring research results to utilities; and
5) to benefit California ratepayers through lower energy costs.

At the same time the organizing committee was forming CIEE, efforts were underway to obtain funding from California utilities and commissions. Funds totalling $1.44M had been secured by the end of FY 1987; however, CIEE had not yet become an organizational entity. An organizational arrangement compatible with CIEE's intended purpose and acceptable to LBL, UERG, and the University of California Office of the President (UCOP) is being developed, and the future of CIEE as an established research institute seems assured.

TESTIMONY

Testifying before congressional committees and before state utility commissions is an important activity of the Center for Building Science. During 1987, testimony was presented before 1) The Subcommittee on Energy and Power of the Committee on Energy and Commerce, U.S. House of Representatives, Washington, DC; 2) The House Budget Committee Task Force on Community and Natural Resources, Washington, D.C.; 3) Subcommittee on Energy Research and Development of the Senate Committee on Energy and Natural Resources, Washington, DC; 4) The Public Service Commission of the District of Columbia, Washington, DC; 5) The Connecticut Department of Public Utility Control, New Britain, CT.

In addition, a comprehensive analysis of demand-side electricity services was prepared for the State of Michigan Department of Commerce and Public Service Commission. These activities are important for promoting energy efficient practices by our nation.

LEAST-COST UTILITY PLANNING

Members of the National Association of Regulatory Utility Commissioners (NARUC) Conservation Committee were invited to Lawrence Berkeley Laboratory for a full day of presentations describing least-cost utility planning (LCUP) research conducted by programs of the Center. Proceedings of the meeting were presented to all attendees. The overall reaction of participants was enthusiastic.

Funding has been obtained to create a LCUP Information Systems Network. This project will update and merge technology databases from such U.S. institutions as EPRI, GRI, and LBL with similar institutions in other countries. A Least-Cost Document Base will also be created that includes regulatory reports from NARUC, electric reports from EPRI, gas reports from GRI, and abstracts of recent papers presented at conferences. These databases will be updated frequently.

INFORMATION TRANSFER

Because the value of energy efficiency research depends on acceptance by many people who do not work in this field, communication of research results is particularly important. For this

reason, a mailing list with 5000 entries was created and a letter asking for an expression of interest in various categories of energy efficiency research was circulated. Six hundred and fifty packets of different kinds of information were mailed to respondants.

PUBLICATIONS

This partial list of publications describes FY87 Center activities. Earlier or more recent publications may be obtained by calling (415) 486-4834.

Rosenfeld A. Conservation, Competition and National Security [Concluding remarks made at the 15th Annual Illinois Energy Conference, University of Illinois at Chicago, November 10-11, 1987.] Strategic Planning and Energy Management Journal 1988; 8(1):530. (LBL-24755b)

Rosenfeld A. Conservation, Competition and National Security. [Testimony for the Hearing on Energy Security: The Role of Conservation in the National Energy Picture; Subcommittee on Energy and Power, Committee on Energy and Commerce, U.S. House of Representatives. Washington, D.C. November 4 1987. (LBL-24755a)

Krause F, Rosenfeld A, Levine M. Analysis of Michigan's Demand-Side Electricity Resources in the Residential Sector Volume I, Executive Summary. Report prepared for the State of Michigan Department of Commerce and Public Service Commission, May 1987. (LBL-23025)

Mills E, Rosenfeld A. Managed Versus Unmanaged 7-Year Electric Growth: Californians Needed 3 New Plants, Texans Needed 11. Excerpted in Physics and Society 1987; 16(2):3-4. (LBL-22932)

Huang J, Akbari H, Taha H, Rosenfeld A. The Potential of Vegetation in Reducing Summer Cooling Loads in Residential Buildings. Journal of Climate and Applied Meteorology 1987; 26(9):1103-1116. (LBL-21291)

Geller H, Harris J, Levine M, Rosenfeld A. The Role of Federal Research and Development in Advancing Energy Efficiency: A $50 Billion Contribution to the US Economy. Annual Review of Energy 1987; 12:357-395.

Rosenfeld A, Geller H, Harris J, Levine M. Federal Research and Development on Energy Efficiency: A $50 Billion Contribution to the U.S. Economy. ASHRAE, ASHRAE Transactions 1987; 93 (Pt. 1):1011-1024.

Rosenfeld A. The Successes of Conservation. Proceedings of the Workshop on Integrated Energy Resources Planning for Electricity on Oahu , Honolulu, HI, May 20-21, 1987, pp. 40-98.

Rosenfeld A, Mills E. The Successes of Conservation. In: de Almeida A, Rosenfeld A (Eds.). Demand-Side Management and Electricity End-Use Efficiency [Proceedings of the NATO Advanced Study Institute, Povoa do Varzim, Portugal, July 20-31, 1987], pp. 17-61.

Krause F, Colborne W, Rosenfeld A. The Potential for Electrical Efficiency in the Residential Sector Case Study Michigan, USA. In: de Almeida and A. Rosenfeld (Eds.). Demand-Side Management and Electricity End-Use Efficiency [Proceedings of the NATO Advanced Study Institute, Povoa do Varzim, Portugal, July 20-31, 1987], pp. 621-642.

ENERGY CONVERSION AND STORAGE

INTRODUCTION

The Energy Conversion and Storage Program has four main projects applying chemistry and chemical engineering to problems in the production of new fuels, their environmental impact, and energy storage and conversion. These projects are:

(1) Electrochemical energy storage and conversion
(2) Thermal energy storage and conversion
(3) Coal-related research
(4) Energy-related chemistry

Each of these projects focuses on transport-process principles, chemical kinetics, thermodynamics, separation processes, and organic and physical chemistry, and advanced analysis methods.

The electrochemical energy storage and conversion project provides research to develop advanced power systems for electric vehicle and stationary energy storage applications. Topics include identification of new electrochemical couples for advanced rechargeable batteries, improvements in battery and fuel cell materials, and the establishment of engineering principles applicable to electrochemical energy storage and conversion. Major emphasis is on applied research that will lead to superior performance and lower life-cycle costs.

The second project is a series of research and development efforts in thermal energy storage and conversion. This project focuses on new and innovative approaches to the more efficient utilization of thermal and solar energy.

The third project involves the development of improved, energy-efficient methods for processing waste streams from synfuel plants and coal gasifiers. Also included in this project is an effort to develop an advanced model of moving-bed coal gasifiers in order to better understand their operation and improve their design.

The last project addresses the identification, characterization, and separation of components in liquid fuel system streams. On-going research topics include the use of advanced methods to remove nitrogen-containing compounds from petroleum feedstocks and wastestreams, the synthesis and characterization of complex organometallic compounds, the development of innovative methods to remove trace heavy metal compounds from fossil materials, and the study of biomimetic reactions to carry out the hydroxylation of hydrocarbons. Novel processes, such as separations by reversible chemical association, are being developed to recover valuable organic products from dilute aqueous solutions that result from the fermentation of biomass. In addition, ultra-sensitive spectroscopic techniques are being applied to detect trace amounts of materials.

ELECTROCHEMICAL ENERGY STORAGE AND CONVERSION

Technology Base Research Project for Electrochemical Energy Storage*

E.J. Cairns, K. Kinoshita, and F.R. McLarnon

The Lawrence Berkeley Laboratory (LBL) is lead center for management of the Technology Base Research (TBR) Project, which is supported by the Electrochemical Branch of DOE's Office of Energy Storage and Distribution. The purpose of this project is to provide the research base to support DOE efforts to develop electrochemical energy conversion systems for electric vehicle and stationary energy storage applications. The specific goal is to identify the most promising electrochemical technologies and transfer them to industry and/or another DOE program for further development and scale-up.

The general research areas addressed by the TBR Project include identification of new electrochemical couples for advanced batteries, determination of technical feasibility of the new couples, improvements in battery components and materials, establishment of engineering principles applicable to electrochemical energy storage and conversion, and the investigation of fuel cell and metal/air systems for transportation applications. Major emphasis of the project is given to applied research that will lead to superior performance and lower life-cycle costs.

The LBL scientists who participate in the project are E.J. Cairns, K. Kinoshita and F.R. McLarnon of the Applied Science Division, and L.C. DeJonghe, J.W. Evans, R.H. Muller, J.S. Newman, P.N. Ross and C.W. Tobias of the Materials and Chemical Sciences Division.

ACCOMPLISHMENTS DURING FY 1987

LBL conducted a vigorous in-house research program and monitored 25 subcontracts during FY 1987. A description of the research projects conducted by the subcontractors can be found in the recent annual report, *Technology Base Research Project for Electrochemical Energy Storage* (LBL-23495), and the in-house work, "Electrochemical Energy Storage," is summarized in the next article and in the *Materials and Chemical Sciences Division 1987 Annual Report* (LBL-24242). Highlights of the subcontracted work follow:

Exploratory Research

- Efforts continue at Argonne National Laboratory (ANL) on testing of 20-Ah $LiAl/FeS_2$ cells containing a dense upper-plateau FeS_2 electrode, a Li-Al electrode, and LiCl-LiBr-KBr electrolyte (m.p. 310°C). The cycle-life stability of cells containing 15-mol% CoS_2 in the positive electrode is being evaluated in an accelerated test. A cell has been operating for over 300 deep discharge cycles with a capacity loss of about 4%. Experiments are now underway to demonstrate overcharge protection of lithium-limited cells.
- Gould, Inc. has focused their efforts on cell design and construction to improve the hermeticity of Li-alloy/FeS_2 cells. A new cell design incorporating a glass-metal feedthrough attached to the cover and an all-welded construction is under evaluation.
- Experimental measurements at the University of Pennsylvania demonstrated that poly(ethylene oxide) [PEO] containing a Mn(II)/Mn(III) redox couple with the composition $(PEO)_nMnBr_2$ (n = 8 or 16) shows interesting properties for use in positive electrodes for ambient-temperature lithium cells.
- The University of Minnesota is investigating the mechanisms of reactions occurring at the electrode/electrolyte interface of novel electrochemical cells containing thin-film polymer electrolytes. Experiments are currently underway on electrodes containing sodium and divalent metals, such as zinc, magnesium and calcium, and PEO electrolyte.
- EIC Laboratories, Inc. has developed a novel low-temperature chemical synthesis method to produce lithium anode materials such as Li-Al, Li_xWO_2, $Li_xFe_2O_3$ and $LiCoO_2$ for rechargeable lithium cells containing organic electrolytes and metal-oxide cathodes.

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Energy Storage and Distribution of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Applied Science Research

- Two major areas of focus of the research project at Stanford University are: (i) develop replacements for the negative electrode/β''-Al_2O_3 assembly in the Na/β''-Al_2O_3/$NaAlCl_4$/$FeCl_2$ (Zebra) cell, and (ii) preparation of thin-layer electrode and electrolyte materials by high-rate atmospheric pressure chemical vapor deposition (CVD) techniques. A combination of sodium alloy electrode and $NaAlEt_4$ (Et = ethyl group) liquid electrolyte appears to be an attractive alternative to the Na /β''-Al_2O_3 assembly in Zebra cells. Initial experiments with the CVD apparatus demonstrated that thin films of $FeS_{1.5}$ can be easily produced.
- ANL has encountered some difficulty in preparing glass tubing from a glass with a composition (42 mol% Na_2O - 8 mol% Al_2O_3 - 5 mol% ZrO_2 - 45 mol% SiO_2) that was previously identified as a candidate solid electrolyte for use in high-temperature Na/S cells. An alternative fabrication process has been recently developed that allows the production of glass tubes of sufficient quality and quantity for sealed-cell testing.
- Massachusetts Institute of Technology has identified glasses with adequate lithium-ion conductivity for battery applications, but improved stability in lithium and sulfur environments is required. Preliminary measurements indicate that calcium-containing lithium borate glasses are stable at high lithium activities.
- The Illinois Institute of Technology (IIT) has successfully electrodeposited Mo and Mo_2C layers from a FLINAK (LiF-NaF-KF) melt. The corrosion rates of these materials in Na_2S_3 melts at 300°C indicates they may be suitable for use as coatings on containment materials in Na/S cells.
- Brookhaven National Laboratory (BNL) has continued EXAFS (Extended X-ray Absorption Fine Structure) studies of zinc bromide electrolytes. Analysis of a dilute electrolyte (0.1 M $ZnBr_2$) indicates that the bromide ions are surrounded by a very loosely bound hydration sheath with a Br-O distance of ~3.0Å. At higher concentration (3 M $ZnBr_2$) only two waters of hydration are associated with the bromide ions.
- The effects of transport processes on the kinetics and morphology of zinc deposition in acidic electrolytes are being investigated by IIT. The propagation of zinc dendrites can be almost completely suppressed at a rotating cylinder electrode (at 400 rpm rotation speed) up to a loading of ~140 mAh/cm^2.
- Surface science methods (thermal desorption, low-energy electron diffraction, work function, Raman) are being applied at Case Western Reserve University (CWRU) and Jackson State University to characterize the surface of reactive alkali and alkaline earth metals in organic electrolytes. Raman spectroscopy indicates that Li_2CO_3 and Li_2O are formed on a lithium surface in propylene carbonate (PC).
- Johns Hopkins University is investigating the corrosion resistance of commercial materials in organic electrolytes. Their studies show that the presence of water in organic electrolyte (0.5 M $LiClO_4$/PC) has a strong influence on the corrosion of Armco steel. As the water content in PC decreases, Armco steel becomes more susceptible to localized attack because it cannot be readily passivated.

Air Systems Research

- Efforts continue at CWRU to develop more effective electrocatalysts for oxygen reduction and generation. The studies indicate that transition metal oxides are active catalysts for oxygen generation and peroxide decomposition, but they have shown poor activity for oxygen reduction in alkaline electrolytes. However, heat treatment of a mixture of a transition metal organic macrocycle (cobalt octaethylporphyrin supported on Vulcan XC-72) and $La_{0.8}Sr_{0.2}Co_{0.9}Ru_{0.1}O_3$ perovskite has shown good activity for oxygen reduction in 4 M NaOH at 60°C.
- Experiments at Pinnacle Research Institute demonstrated that further improvement in the discharge performance of zinc/air cells with flowing electrolyte is possible with the use of a combination of additives. The addition of 25 g/l silicate (SiO_2) + 15 g/l sorbitol to 12 M KOH increased the zinc capacity from 87.2 Ah/l to 191.3 Ah/l and the zinc utilization (300 g/l initially at full charge) from 35.45 to 77.79% at a discharge current density of 200 mA/cm^2.
- Experiments are underway at SRI International to investigate the rate and mechanism of aluminum corrosion in KOH electrolyte in Al/air batteries. Aluminum alloys containing Li and In were found to exhibit quite negative potentials (to -1.755 V versus Hg/HgO) but also displayed high corrosion rates (260-340

mA/cm^2). Alloys containing In, Mg and Mn also exhibited negative potentials (-1.790 to -1.820 V), but showed somewhat lower corrosion rates (75 to 118 mA/cm^2).

- Los Alamos National Laboratory (LANL) has improved the fabrication process for air electrodes in proton-exchange membrane (PEM) fuel cells. By optimizing the hot pressing conditions used to fabricate the Prototech electrode and Nafion membrane structure, and increasing the surface concentration of Pt by sputtering a thin film of Pt onto the structure, a significant improvement in performance at current densities to 1 A/cm^2 was observed. These results demonstrate that mass-transport limitations in PEM fuel cells can be greatly reduced.
- EXAFS was utilized by BNL to characterize heat-treated macrocycles (cobalt and iron tetramethoxyphenyl porphyrins (TMPP)) for O_2 reduction in fuel cells. For Fe-TMPP supported on Vulcan XC-72, EXAFS revealed that a FeN_4 structure remained after heat treatment at 900 and 1000°C. This type of moiety was reported in independent studies by CWRU to be active for O_2 reduction.

PROGRAM CHANGES IN 1987

Funding support for the following project was initiated in 1987:

- Development of Anode Alloys for Aluminum/Air Batteries – SRI International.

The following work was completed in 1987:

- Ambient-Temperature Secondary Lithium Batteries Using LiAl or Lithium Insertion Anodes – EIC Laboratories, Inc.
- Transport in Aqueous Battery Systems – Lawrence Livermore National Laboratory.
- Aluminum/Air Power Cell Research and Development – Lawrence Livermore National Laboratory.

PLANNED ACTIVITIES FOR FY 1988

New initiatives include the following:

- Zinc/Air Battery R&D.
- *In Situ* Studies of Electrode Surfaces.

Advanced Electrode Research*†

E.J. Cairns, F.R. McLarnon, T.C. Adler, M.J. Isaacson, K.G. Miller, S.A. Naftel, J. Rudnicki, and K.A. Striebel

The purpose of this research is to study the behavior of electrodes used in secondary batteries and fuel cells, and to investigate practical means for improving their performance and lifetime. Systems of current interest include ambient-temperature rechargeable cells with Zn electrodes (Zn/air, Zn/NiOOH, Zn/AgO, Zn/Cl_2, Zn/Br_2, and Zn/$Fe(CN)_6^{-3}$); rechargeable high-temperature cells (Li/S, Li-Al/FeS_2, Li-Si/FeS_2, and Na/S); fuel cells; and liquid-junction photovoltaic cells. The approach used in this investigation is to study life- and performance-limiting phenomena under realistic cell operating conditions.

ACCOMPLISHMENTS DURING FY 1987

ALKALINE ZINC ELECTRODES

Rechargeable alkaline Zn/air and Zn/NiOOH cells can be designed to deliver high specific energy and specific power, but they typically exhibit short lifetimes. The high solubility of Zn species in alkaline electrolytes tends to enhance the various physiochemical processes (active material redistribution, filamentary Zn growths, etc.) which degrade the cell's capacity and limit its life. Modeling and experimental investigations are aimed at understanding the

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Energy Storage and Distribution of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

†This project is part of a larger effort, "Electrochemical Energy Storage," described in the Materials and Chemical Sciences Division 1987 Annual Report (LBL-24242).

complex transport processes in operating Zn electrodes, and characterizing various methods to reduce Zn species solubility and extend the lifetime of the Zn electrode.

Measurement of Concentrations in Porous Zinc Electrodes Using Micro-Electrodes

(M.J. Isaacson, E.J. Cairns and F.R. McLarnon)

Zn and Cd μ-electrodes have been used to investigate processes in cycling porous Zn electrodes.[1] Electrodes were cycled for 30 to 60 cycles in the 17% and 30% KOH. The active material tended to redistribute towards the center of the electrode in cells with 17% KOH electrolyte, and toward the edges of the electrode in 30% KOH electrolyte, as was previously observed in this laboratory.[2]

During the first 20 to 30 cycles the Zn and the Cd μ-electrode potentials changed very little as the electrode was charged and discharged. The potential differences between the μ-electrodes were usually only about 2-4 mV at any particular time, although they changed by about 10-20 mV during a cycle. Surprisingly, a potential minimum was frequently observed near the beginning of a charge. Small potential gradients were observed at the edge of the electrode in the 17% cell, which correlated well with the position of the edge of the electrode. It was not apparent whether the potential gradients were due to secondary current distribution or to a decrease in the porosity near the electrode edge as material moved toward the center of the electrode.

As cycling continued "structure" started to develop in the Zn μ-electrode data, as seen in Fig. 1. The Cd μ-electrodes also showed an increase in polarization but to a much smaller extent, and later during the cycling than the Zn μ-electrodes. Calculated molalities showed that the increase in μ-electrode polarization was almost entirely due to changes in the $Zn(OH)_4^{2-}$ concentration, which often decreased to 10% of the nominal concentration during charge and increased to 300% of the nominal concentration during discharge. X-ray photographs of the electrodes indicated that the largest changes in the μ-electrode potentials and concentrations occurred in areas which may have experienced an increase in current density due to material redistribution.

The μ-electrode potentials and molalities indicate that the electrode is not limited by transport of reactants and products in early cycles. However as cycling continues and material redistribution occurs the electrode becomes limited by transport of

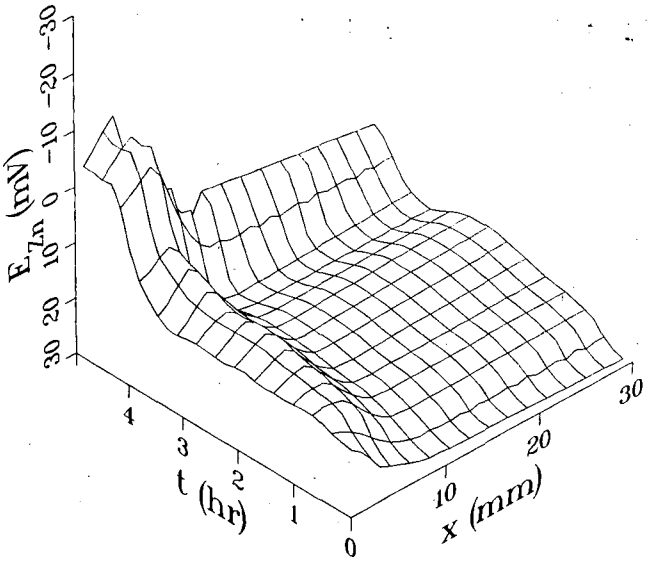

Figure 1. Zn μ-electrode potentials during charge cycle 32 in 30% KOH electrolyte. (XBL 882-577)

$Zn(OH)_4^{2-}$, dissolution of ZnO, or precipitation of $Zn(OH)_4^{2-}$. This limitation is probably due to an increase in the current density and a decrease in the electrode porosity in areas where the μ-electrode polarization is increasing.

Mathematical Modeling of the Zinc Electrode

(K.G. Miller, E.J. Cairns and F.R. McLarnon)

The one-dimensional, time-dependent model reported earlier[3] has now been implemented.[4] This model is designed to elucidate the the cause of active material redistribution in the Zn electrode, and it takes into account transport of electrolyte species, heterogeneous reactions, kinetics, and current density variations.

A simplified version of this model, where the concentration terms are omitted from the equations for Ohm's Law in the electrolyte phase and the electrolyte velocity is assumed to be zero, provides insight into the transient electrolyte changes over the course of one cycle. The results for the changes in the concentrations of zincate ion ($Zn(OH)_4^{2-}$) and hydroxide ion (OH^-) are shown for both Zn and Ni electrode compartments for one cycle (5.0 hour charge, 15 minute open-circuit, 2.5 hour discharge) in Fig. 2. The concentrations represent a particular location in the center of the cell. The results were found to be very sensitive to the value of the precipitation/dissolution rate constants, and the values used in the results presented here were both

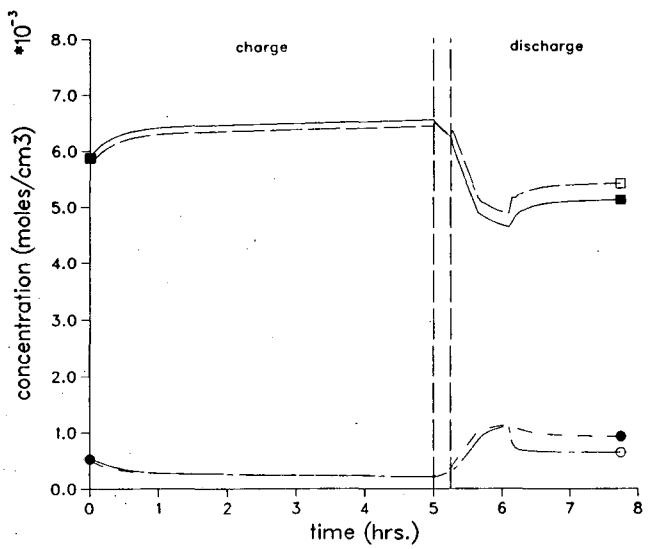

Figure 2. Calculated concentrations from Zn/NiOOH cell model for one cycle (5.0-hour charge, 15-minute open-circuit, 2.5-hour discharge). The precipitation/dissolution rate is 2.5×10^{-5} cm/sec. These concentrations are at a particular location in the middle of the cell. Symbols represents concentrations as follows: ■, OH^- in the Zn compartment; □, OH^- in the Ni compartment; ●, $Zn(OH)_4^{2-}$ in the Zn compartment; ○, $Zn(OH)_4^{2-}$ in the Ni compartment. (XBL 882-578)

2.5×10^{-5} cm/sec. Another important point concerns the onset of precipitation or dissolution of ZnO. Experimentally, it has been found that when a KOH solution is undersaturated with $Zn(OH)_4^{2-}$, ZnO will always dissolve. However, during discharge, it has been found the electrolyte can supersaturate to about three times the equilibrium concentration of $Zn(OH)_4^{2-}$. Therefore, the model was developed so that whenever the electrolyte was undersaturated, dissolution of ZnO always occurred. When the electrolyte became supersaturated in $Zn(OH)_4^{2-}$, precipitation was not allowed to occur until the concentration of $Zn(OH)_4^{2-}$ was three times its saturation value. The following trends have been found from the model:

(1) By the end of the charge cycle, the concentration of OH^- increases only about 15% whereas the concentration of $Zn(OH)_4^{2-}$ decreases by about a factor of 50% from their initial values.

(2) The differences in concentrations of both $Zn(OH)_4^{2-}$ and OH^- in the Zn and NiOOH electrode compartments are not very large during charge. This shows there is good movement from one side of the microporous separator to the other.

(3) During discharge, the concentrations of both $Zn(OH)_4^{2-}$ and OH^- change much more than during the charge cycle. This is due to supersaturation of the electrolyte with $Zn(OH)_4^{2-}$. After precipitation of zincate (as ZnO) occurs the concentrations remain relatively unchanged. Also, the concentration differences between the Zn and Ni electrode compartments are much greater after precipitation starts, during discharge. This could be explained by the fact that the precipitation of zincate (as ZnO) was observed to be faster in the Zn compartment due to the higher concentration of $Zn(OH)_4^{2-}$ in the Zn compartment than in the Ni compartment.

In addition, the model was run at different rates of precipitation/dissolution to see what effect this parameter had on the results. During charge, if the value was set at 5.0×10^{-5} cm/sec, there was very little change in the concentrations of both $Zn(OH)_4^{2-}$ and OH^- from their initial values. However, if the rate was set at 1.5×10^{-5} cm/sec, the concentration of $Zn(OH)_4^{2-}$ dropped nearly to zero by the end of charge. This demonstrates that there is only a narrow value of this parameter that gives meaningful results.

Investigations of Methods to Improve Zinc/Nickel Oxide Cell Lifetime

(T.C. Adler, F.R. McLarnon, and E.J. Cairns)

Three factors under investigation for improving Zn/NiOOH cell cycle-life performance are: 1) electrolyte composition,[2] 2) electrode composition,[5] and 3) charging method.[6] Zn/NiOOH cells using 25-33 mol% $Ca(OH)_2$-additive in the Zn electrodes, 31 wt% KOH or 15 wt% KOH-15 wt% KF electrolytes, and a 30-ms on/90-ms off pulse-charging regimen were investigated.[7] Although one of these cells lasted for over 500 cycles, they generally failed from dendritic shorting within 20-60 cycles. The $Ca(OH)_2$-additive electrodes cycled in 31 wt% KOH exhibited diamond-shaped crystals characteristic of $CaZn(OH)_4$. No such crystals were observed in $Ca(OH)_2$ additive electrodes cycled in KOH-KF electrolyte because CaF_2 is thermodynamically favored over $CaZn(OH)_4$. An electrode of pure $CaZn(OH)_4$ cycled at constant current in 31 wt% KOH was well-behaved and showed a very uniform distribution of material after 50 cycles, much better than observed with the $Ca(OH)_2$-additive electrodes. Cells containing negative electrodes of ZnS and ZnSe, having very low solubilities in 31 wt% KOH, produced very high

overpotentials on formation, along with low charging efficiencies. Several new separator materials were evaluated, but none of them provided a superior barrier to dendrite penetration, as compared to three layers of microporous polypropylene (Celgard).

The cells described above transferred Zn to the NiOOH electrode at the same rate as standard Zn-electrode cells. An average of 45% of the weight gained by the Ni electrode during cycling was present as Zn, consistent with the interpretation that Zn ions displaced Ni ions in the α-nickel hydroxide hydrate of the Ni electrode. Impregnating the NiOOH electrode with ZnO prior to cycling might slow the rapid transfer of Zn to the NiOOH electrode in the early cycling of the cell, and allow the Zn electrode to be reduced in weight, maintaining satisfactory specific energy. Mechanical deposition of ZnO from an aqueous slurry into the NiOOH electrode on a vacuum table loaded only about one-fourth the amount required, so this may need to be carried out by an electrochemical process.

The computer-controlled cell cycling system is being modified for charging cells in a constant-voltage, limited-current mode which prevents the occurrence of high overpotentials associated with the formation of Zn dendrites.

HIGH-TEMPERATURE CELLS

The high-temperature Na/S cell offers very good performance, and recent improvements to the process for manufacturing the ceramic β''-Al_2O_3 electrolytes indicate that acceptable cell lifetimes may be realized. However, the performance of the sulfur electrode has not been optimized, and the phenomena which govern its operation are poorly understood. On-going work is aimed at developing and confirming an advanced mathematical model of the sulfur electrode.

Mathematical Modeling of the Sodium/Sulfur Cell

(S.A. Naftel, F.R. McLarnon and E.J. Cairns)

A comprehensive model of the sulfur electrode in Na/S cells has been developed.[8,9] The cell being modeled is of the tubular central-sodium type, and includes a thin layer of α-alumina felt around the β''-alumina solid electrolyte,[10,11] in order to prevent deposition of sulfur on the solid electrolyte during cell charge. The model consists of a set of non-linear PDE's which describes the processes of diffusion, migration, and convection which take place during the operation of such a cell. Solution of the linearized equations is effected on a digital computer via implementation of the Newman-IAD method,[12] a finite-difference technique for the solution of second order linear PDE's.

Fluid flow through the sulfur electrode, which is essentially a porous graphite felt, is accounted for by use of the differential form of Darcy's law, $v = k\nabla P$, for flow through porous media. This requires the use of capillary pressure and relative permeability, both of which are functions of the fluid-matrix system.[13] Due to the difficulty of performing measurements on the sulfur/polysulfide/graphite system directly, an analogous system (water/bromobenzene/glass fiber) was used. Theory[14] was then applied in order to estimate the capillary pressure and relative permeability values for the system of interest, using the experimental data. Figure 3 shows the relative permeability of the sulfur (wetting) and polysulfide (non-wetting) phases as functions of the saturation (volume fraction). Beyond a value of saturation of 0.75, the polysulfide phase is no longer interconnected, and it does not

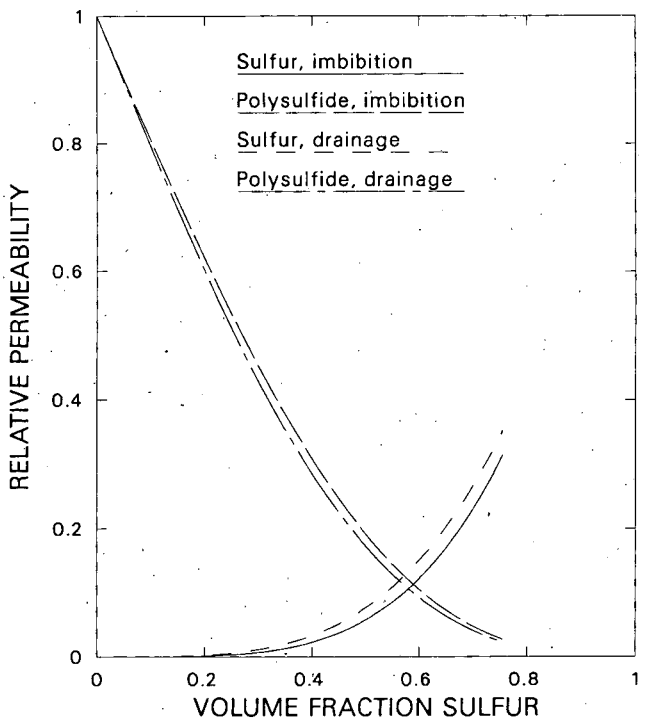

Figure 3. Computed values of relative permeability of sulfur and sodium polysulfide in graphite felt. Values are shown for both the imbibition(displacement of polysulfide by sulfur), and the drainage(replacement of sulfur by polysulfide) cycles. Beyond a sulfur volume fraction of 0.78, the polysulfide phase is discontinuous and no longer moves. (XBL 882-579)

move. The relative permeabilities of the sulfur and polysulfide phases are 1 and 0 respectively in this region. The only other physical property remaining to be measured is the graphite felt conductivity. All other physical properties are available in the literature.

The results of this modeling will be compared with data from an operating cell which has been designed to allow measurement of ionic potentials throughout the sulfur electrode. An attempt will be made to predict the effect of various charge-discharge regimens upon cell operation.

FUEL CELLS

Fuel cells can be designed to exhibit acceptable lifetimes for a number of applications. However, the performance of the O_2 electrode in fuel cells requires improvement, and the development of an efficient direct-methanol fuel cell would represent a major advance over reformed-hydrocarbon fuel cells.

Application of PDS to Electrochemical Interfaces

(J. Rudnicki, E.J. Cairns and F.R. McLarnon)

Photothermal deflection spectroscopy (PDS) has been developed as a sensitive *in-situ* method for investigation of electrochemical interfaces.[15-17] This method is a novel application of PDS, and should prove to be an exceptional addition to the few *in-situ* techniques currently in use. An advantage of this technique is that the electrode surface is not required to be optically smooth. The same system is also used to simultaneously measure concentration gradients adjacent to the electrode surface. This additional information is helpful in determining the surface chemistry. Various types of electrochemical interfaces can be studied by this method, e.g., corrosion, secondary electrodes, and electrocatalysts. The objective of this work is to study direct electro-oxidation of methanol on Pt ad-atom catalysts. Increased understanding of these catalysts will aid in the development of high-performance direct methanol-air fuel cell systems.

PDS is a comparatively simple system. Monochromatic light is directed through the electrolyte and onto the electrode at a normal incidence. Absorption of light by the surface causes heating of the electrode and thereby forms a thermal gradient adjacent to the electrode. Index of refraction is a function of temperature; an associated gradient in the index of refraction is formed. A probe laser beam is directed parallel to the electrode through this gradient and is deflected. The magnitude of this deflection is proportional to the surface absorption. Modulation of the light source and lock-in detection are implemented to increase the signal-to-noise ratio.

Electrochemical reactions will create concentration and associated refractive-index gradients, which can be measured by the probe beam. Since this deflection is not modulated, it can be discriminated from the deflection due to the surface absorption by the lock-in instrumentation, yielding simultaneous measurement of surface absorption and concentration gradients.

The primary parameter measured by PDS is the absorption of light at a surface. Scanning of the wavelength of the source allows spectra of the interfacial species to be obtained. Confirmation experiments on systems with known spectra have been successful. Absorption can be measured at constant wavelength while the electrode potential is changed. Cyclic voltammetry of Pt in 0.1 M $HClO_4$ along with the corresponding absorption and concentration gradient is shown in Fig. 4. This experiment shows that PDS is sensitive to the formation of single layers of molecules at the surface; in this case, the formation of platinum oxide is clearly seen. The microscopic concentration gradients formed are also evident.

Preliminary experiments on the oxidation of methanol on Pt and an under-potential deposition (UPD) process by which ad-atom catalysts are formed have shown that PDS will be an effective tool to increase the understanding of these systems. Developmental effort is under way to extend the spectral range of the system into the infra-red. This would allow *in-situ* vibrational spectra to be obtained, which can help identify organic surface species.

Oxygen Reduction In Alkaline Fuel Cell Electrolytes

(K.A. Striebel, E.J. Cairns and F.R. McLarnon)

Voltage losses in the O_2 cathode represent the major inefficiency in aqueous fuel cells for transportation or stationary applications. Experimental and theoretical studies of oxygen reduction (OR) in aqueous alkaline electrolytes on smooth and supported Pt have been carried out.[18,19]

The mechanism for OR on Pt in alkaline electrolytes is complicated by the concurrent oxidation and reduction of Pt. Rotating ring-disk electrode (RRDE) studies carried out with anodic and cathodic potential sweeps in 0.1 to 6.9 M KOH and 0.1 to 4.0 M

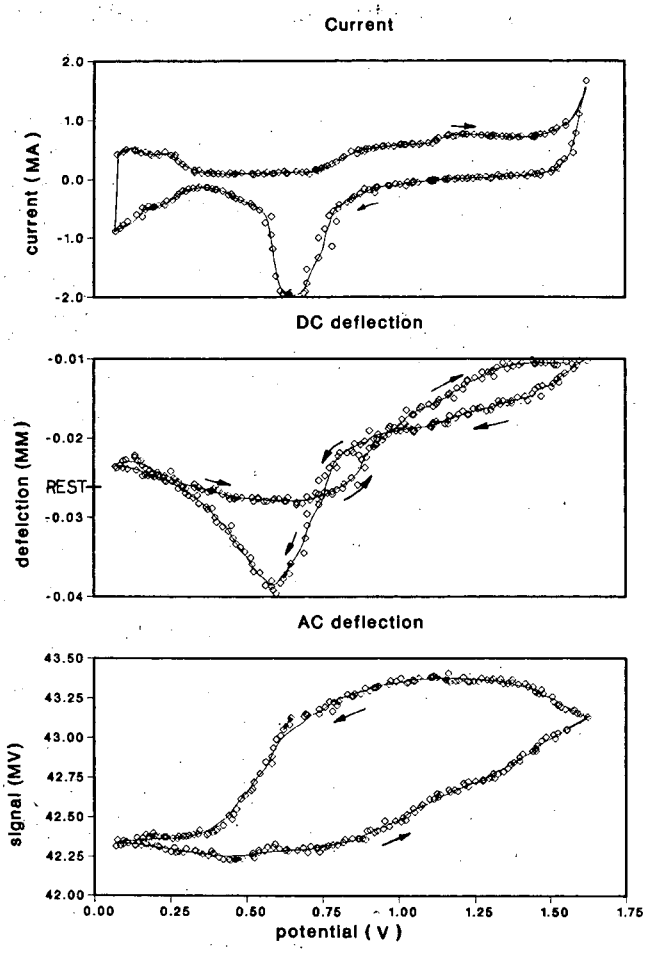

Figure 4. Simultaneous cyclic voltammetry and PDS of Pt in 0.1 M $HClO_4$. The upper plot shows the electrode current response to a cyclic potential scan at 100 mV/s. The DC deflection lot represents the concentration gradients formed in the electrolyte. Deflections positive to the REST deflection indicate that the electrolyte concentration near the electrode is higher than in the bulk, and deflections negative to the REST deflection indicate lower electrolyte concentrations. The AC deflection plot indicates the amount of light absorption at the electrode surface. The excitation light wavelength was 550 nm. (XBL 882-580)

K_2CO_3 revealed similar currents when corrected for O_2 solubility differences. In dilute electrolytes, OR proceeds primarily through the 4-electron pathway to water, independent of pH. In KOH, the mechanism for Pt oxidation changes and the fraction of current yielding a peroxide product increases at 2 to 3 M. These changes were not observed in K_2CO_3.

Porous gas diffusion electrodes (GDE) with supported Pt catalyst were studied in a special cell with low uncompensated solution resistance. Cyclic voltammograms yielded measurements of the wetted areas of carbon and Pt and the local electrolyte composition. GDE galvanostatic steady-state performance with 100% O_2 was measured in 2 to 11 M KOH and 2 to 5.5 M K_2CO_3. Comparisons with kinetic results suggest that OR on carbon contributes to the high currents in 6.9 M KOH at high overpotentials. In K_2CO_3, lower wetted areas and slow OH^- ion transport are responsible for the poor performance when compared with KOH.

Models for the steady-state operation of porous GDE's were developed. These models account for the diffusion and reaction of O_2 and ionic transport in KOH and K_2CO_3. Performance data showed good agreement with the model, using reasonable values for the electrode structural parameters. The non-kinetic Tafel slope and the half-order dependence on O_2 pressure, observed with K_2CO_3, were predicted without using adjustable parameters. Comparison between the model and experiment is shown in Fig. 5. The results suggest that modifications of the GDE structure will be necessary to obtain good performance with aqueous carbonate electrolytes.

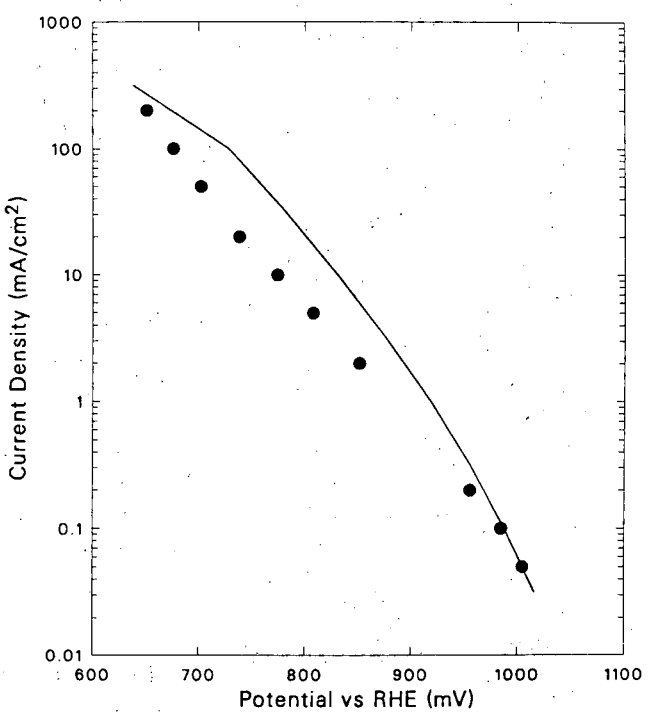

Figure 5. Steady-state model fit to oxygen cathode data recorded in 2M K_2CO_3 electrolyte at 25°C with 1 atm. O_2. (XBL-8711-4714)

PLANNED ACTIVITIES FOR FY 1988

Continuing research efforts on secondary alkaline Zn electrodes will include the cycle-life testing of promising electrode/electrolyte formulations in model cells. An improved mathematical model of the Zn electrode will be fully developed, and cycle-life experiments to verify key features of the model, using *in-situ* microelectrode potential measurements to determine electrolyte species concentrations, will be completed. Optical microscopy and new *in-situ* spectroscopic techniques will be applied to identify the transient species formed during secondary Zn-electrode operation.

A time-dependent, two-dimensional mathematical model of the high-temperature sulfur electrode will be fully developed, and Na/S cell tests will be completed to verify important aspects of the model.

Experiments using porous gas-diffusion electrodes to study O_2 reduction in alkaline-carbonate electrolytes will be completed, and new ad-atom electrocatalysts for high-performance fuel-cell systems will be investigated.

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Direct Solar Thermal Conversion Processes*

A. Hunt, I. Hodara, F. Miller, and J. Noring

In this research area we are exploring advanced concepts in the direct conversion of concentrated solar energy to thermal and chemical forms. Of the four research areas, two involve purely solar thermal processes; the others address the solar heating of catalysts to drive useful chemical reactions. The unifying themes to this research are the study of the absorption of concentrated solar energy by small particles or other microstructures, and the conversion of that energy to other forms. This approach may be applied to heat gases to high temperatures for driving turbogenerators and supplying industrial process heat,[1] or to convert solar energy to chemical forms suitable for storage or transport.[2,3] The concept of entrained particle absorbers was first demonstrated in 1982 with the solar test of the Small Particle Heat Exchange Receiver (SPHER). The test showed that air could be heated to high temperatures by absorption of entrained carbon particles that subsequently oxidized to leave a clear gas stream suitable to power a gas turbine. In the past year we continued to explore new concepts and applications in chemical and thermal solar receivers.

ACCOMPLISHMENTS DURING FY 1987

DIRECT RADIANT HEATING OF GASES BY PARTICLE SUSPENSIONS

This research was undertaken to improve the quantitative understanding of the thermal and optical processes during the radiant heating of gas-particle mixtures. In previous studies, we developed methods to calculate the solar absorption by the particles and determine the heating rates and temperatures of the gas and particles. In FY 1987 we continued development of a cylindrical receiver model and initiated experimental work to study the operation of a complete receiver system. The goal is to understand the complex interactions involved in the absorption of sunlight by the particles, the heating and expansion of the gas, and the resulting temperature, density, and flux profiles within a solar receiver. The results of the research will provide a basis to design future direct absorption receivers.

An analytical model of a long cylindrical receiver was developed to predict the temperature and flux distribution in a gas particle suspension flowing along its axis. The model uses a four-flux radiant transfer approximation that includes absorption, emission, and scattering by the particles, expansion of the gas, and convective and radiant heat transfer. The model provides general information regarding particle densities and the effects of flow direction. It also provides detailed performance predictions of our experimental receiver.

An experimental receiver system was designed and constructed to test the model. The experimental system consists of a vacuum-insulated cylindrical (.05 x 1 m) receiver, carbon particle generator, light source, and associated instrumentation. The light source produces a collimated beam of light along the axis of the tube with a peak intensity of over 80 suns. Carbon particles produced by the pyrolysis of C_2H_2 are mixed with air and directed in either a co- or counter-current flow direction with respect to the direction of the incident light. Thermocouples measure the temperature profile along the entire axis at 6 different radial positions and at fixed points within the receiver. The mixture opacity is monitored with laser transmissometers at 3 axial positions, and the total flux reaching the end is monitored. The receiver will be completed in FY 1988 and the measurements will be compared with the model predictions.

CARBON PARTICLE ABSORBERS IN LIQUID SALTS

The DOE Central Receiver Program is developing an advanced direct absorption receiver based on a liquid nitrate salt heat transfer and storage medium. The salt flows over a plate exposed to concentrated solar radiation from a field of heliostats. Because the pure salt is transparent to solar radiation, current designs call for the salt to be doped

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with cobalt oxide particles. In this second solar thermal concept we are investigating the use of carbon particles as an alternative absorber. Carbon particles are less abrasive and are slowly oxidized in the hot salt. The oxidation of the particles effectively eliminates problems of agglomeration and settling encountered with the cobalt oxide particles.

The study investigated the dispersion and oxidation of carbon particles in liquid Na/K nitrate salt. Experiments were run on 11 different types of carbon to study the ease of dispersal and the time to complete oxidation. Spectroscopic analysis of the salt after the experiments indicated that the carbon was oxidized to carbon monoxide, reducing the formation of undesirable nitrites. The carbon takes typically up to one hour to oxidize, meaning the rate of CO release to the air is very slow.

In addition to the experimental work, calculations were performed using a solar absorption model based on the Mie theory of scattering to determine the mass loading of carbon and cobalt oxide required to produce the necessary absorption in a path length of a few millimeters. These calculations showed that carbon was a better absorber on a weight basis than cobalt oxide. The work will continue in FY 1988 with a technical and economic assessment of the merits of the two absorbing agents.

RADIANTLY HEATED CATALYSTS FOR THERMOCHEMICAL ENERGY STORAGE

This work investigates the use of concentrated sunlight to directly initiate endothermic catalytic reactions in gases. This approach has application to high-temperature energy storage cycles using thermochemical reactions. Direct radiant heating of catalyst particles to drive endothermic reactions in gases offers significant advantages over traditional catalyst heating methods. These advantages include enhanced heat transfer because the heat is supplied directly to the site of the reaction. In conventional catalytic reactors, heat is supplied through pipe walls and to the reaction site by conduction and convection, leaving the catalyst the coolest part of the system. When a light-absorbing catalyst is radiantly heated it is the hottest part of the reactor, dramatically increasing the rate of reaction. Secondly, a semiconducting particle may photocatalyze the reaction because photons absorbed in semiconducting particles can produce energetic photocharges. In small particles these charges can reach the gases adsorbed on the surface and participate in the reaction.

We have studied the endothermic dissociation of SO_3 to SO_2 and O_2 as a vehicle for thermochemical storage of solar energy. This reaction occurs over a catalyst at 800 to 900°C. Experiments with hematite (iron oxide) particles fixed on a substrate and illuminated with a solar simulator showed large enhancements in dissociation rate. However, the SO_3 storage and transfer system was difficult to maintain because of the reactivity of the sulfur compounds. In addition, the reaction cell design caused uncertainty in the interpretation of the results. This year the SO_3 storage and transfer system was competely redesigned. A new reaction cell will be fabricated and the system assembled in FY 1988 for a new series of experiments.

RADIANTLY HEATED CATALYSTS FOR ENERGY TRANSPORT

A project was initiated to study the feasibility of direct radiant reactors for the chemical transport of energy. In this concept, parabolic dishes individually concentrate solar energy that is converted to chemical energy and piped as an energy-rich gas to a central site. The gases then pass over a catalyst to produce high-temperature heat to drive a steam-Rankine cycle. A similar process can also be used with central-receiver technology to transport energy for considerable distances. This approach is being explored in collaborative programs with Germany and Israel.

We are studying the feasibility of several types of direct radiant reactors for the CO_2 reforming of methane. CO_2 is reacted with methane over a catalyst at high temperature to produce H_2 and CO. Heat exchangers cool the gas to ambient temperature before it is piped to a central conversion site. Our investigation is analyzing several types of radiantly heated catalytic reactors with respect to operating characteristics and costs.

In all the receiver/reactor designs considered, solar flux was concentrated directly onto a catalyst immersed in the reacting gases. The catalyst was either arrayed on a non-absorbing substrate, or was entrained in the gas. The substrates considered included reticulated alumina, alumina aerogel, and fiber arrays. The fixed catalyst was chosen to be rhodium particles, which if very small become good solar absorbers. Analyses were carried out of the mass transport, optical and thermal properties of the reactor designs.

To aid in comparing the receiver designs, we developed a system model to study the first and second law efficiencies of the entire system.

PLANNED ACTIVITIES FOR FY 1988

Specific goals of the FY 1988 research include experimental validation of the gas-particle receiver model; characterization of the optical properties as well as the oxidation, agglomeration and settling of carbon particles in salt; quantification of the effects of radiant heating on the reaction rate of the dissociation of SO_3; and the development of integrated optical and thermochemical models of radiantly heated catalysts and their supports.

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Microstructured Materials*

A. Hunt, F. Hibbler, P. Hsuin, and K. Lofftus

The goal of this work is to develop new microstructured materials using purely chemical techniques. Liquid organo-metallic compounds are combined with water, solvents, and catalysts to form a gel network that contains solvent. The solvent is removed without changing the microstructure by using a supercritical drying technique developed at LBL. The result is a low-density, porous solid called aerogel. A variety of single- or mixed-oxide compositions can be made this way depending on the starting compounds. Two projects are exploring this technique; one is developing silica aerogel for insulating windows, and the other is exploring the preparation of new ceramic materials.

ACCOMPLISHMENTS DURING FY 1987

SILICA AEROGEL, A TRANSPARENT HIGH-PERFORMANCE INSULATOR

Silica aerogel is a transparent, porous solid that is useful for a wide variety of applications. We are developing silica aerogel as a transparent insulator between double glazings for a high-thermal-performance window or solar collector cover. Such windows will increase the thermal resistance of conventional double glazing by a factor of 5 or more. Recent progress in improving the properties of silica aerogel, and the results of scale-up and technology-transfer activities are described.

Light passes through aerogel with essentially no distortion, but its microstructure scatters a small amount of blue light. We have been working to reduce this residual scattering to the point of acceptability for view glazings. Extensive experiments were carried out in the preparation of alcogel (the aerogel precursor) to determine the clearest formulation. A polarization nephelometer was used to quantify the light scattering from the alcogels. A rather remarkable result of the study was that, within the compositions investigated, the clarity was strongly correlated to the time to gellation.[1] The optimum aerogel density and catalyst content (over the range investigated) was determined to minimize scattering.

A new large autoclave capable of accommodating samples as large 12 inches square was designed and fabricated to carry out the CO_2 substitution and supercritical drying process developed at LBL. Instrumentation for monitoring the fluid level and composition in the autoclave was developed and tested. The first aerogel samples will be dried in the larger autoclave during FY 1988.

Cost studies were carried out that confirmed that aerogel could be produced for a reasonable cost ($\$10\text{-}15/m^2$). The energy savings from using aerogel provide cost paybacks in less than two years in cold climates. Encouraged by the DOE technology transfer program, a company was founded to commercialize the manufacture of aerogel products in the United States using the CO_2 substitution process.

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POROUS MICROMATERIALS DEVELOPMENT

Micromaterials research at LBL is developing new methods to produce microporous materials and precursors based on sol-gel chemistry and supercritical solvent extraction techniques. These techniques have enabled us to create new and unusual materials. Low-density materials with controlled microporosity promise applications including high-temperature insulators, ceramic precursors, and porous materials for filters, membranes, and catalyst substrates.

During FY 1987 we developed preparation methods for single and mixed oxide ceramic materials, initiated research into using sol-gel processing for preparation of high-T_c superconductors, and explored the preparation of organic gels. We studied the colloid chemistry involved in combining sols of alumina with silica. An aerogel with a composition corresponding to mullite (a widely used high-temperature ceramic) was prepared. Sintering tests showed that mullite aerogels sintered at significantly lower temperatures than conventional ceramic processing.[3] This is an important advantage in preparing ceramic composites because the components often react with each other at normal sintering temperatures. In addition to lowering sintering temperatures, the ultrafine aerogel microstructure results in a homogeneous material to near atomic scale.

After an extensive experimental search, we discovered a technique to prepare zirconia alcogels useful for making high-temperature insulators and porous electrodes. We also explored the preparation of mixed ceramic oxides for high-T_c superconductors. As a first step, we explored transesterifacation methods to prepare liquid copper alkoxide starting compounds. YBa_2Cu_{7-x} aerogels may offer significant advantages because the lowered sintering temperature can avoid undesirable phase transitions encountered at normal processing temperatures and the porous structure allows easy oxygen transport.

PLANNED ACTIVITIES FOR 1988

In the silica aerogel research we will concentrate on producing large aerogel tiles for evaluation by industry and encourage the commercial development of aerogel windows and skylights through technology transfer activities. The porous micromaterials area will explore the preparation of transparent dense alumina by sintering aerogel precursors, continue to develop preparation methods for zirconia aerogels, and explore the preparation of copper and mixed-oxide aerogels for high-T_c superconductors.

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Light Scattering Studies*

As part of the study of the interaction of light with microstructures, we have established a capability to carry out basic studies of light scattering. Light scattering is an essential tool in our solar thermal conversion and microstructured materials studies. We are also investigating two topics in the biological sciences. Both involve the detection of specific and unusual effects of scattered light in either live populations or immobilized single cells.

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ACCOMPLISHMENTS DURING FY 1987

OPTICAL MEASUREMENTS OF THE INTRACELLULAR POLYMERIZATION OF HbS

A. Hunt, C. Gross, K. Lofftus, and A. Quintanilha

A new, real-time technique we have developed measures the kinetics of intracellular polymerization of sickle cell hemoglobin. Previously, it was difficult to distinguish polymerization from shape changes in the cell and to quantify polymerization caused by de-oxygenation, hypertonic stress, acidification, or temperature increase. Time-dependent measurements

of the effects of these stresses are important because kinetics plays a key role in the physiological processes that lead to crises in sickle cell patients. We have shown that measurements using a polarization-sensitive light-scattering technique[1] can detect and quantify hemoglobin polymerization.[2] Further, the technique clearly distinguishes polymerization from changes induced in the shape or volume of the cells. The technique is extremely sensitive, allowing studies with very small sample volumes, an important advantage when working with sickle blood.

In a series of measurements on blood of juvenile sickle patients, the normalized induced circular polarized light, measured as a function of angle, changed by 1.5% in a reversible manner when the O_2 content alternatively varied from 7.5 to 0.5 ppm. The current instrumental resolution is about 0.2%. Further, blood from non-sickle patients showed no change within experimental uncertainty under similar experimental conditions. We are currently using this technique to study the kinetics of sickling behavior and how it correlates to perturbations of membrane transport phenomena.

MODELING BIOLOGICAL PARTICLES TO PREDICT OPTICAL PROPERTIES OF THE OCEAN

A. Hunt, M. Quinby-Hunt, F. Livolant, K. Lofftus, and M. Maestre

The objective of this project, begun in June of 1987, is to predict the scattering behavior of the ocean through a modeling program and to evaluate the effects of that scattering on oceanic visibility and irradiance. The largest and most variable component of oceanic scattering arises from particles suspended in the ocean. The organisms can be identified as members of groups, which are *self-similar* and can be described as simple geometric forms or combinations of them. Therefore, it is possible to predict the scattering from such organisms by applying one or more scattering theories depending on the size, internal and external structure, refractive index, and absorptive properties of the organism.[3]

A series of models was implemented as computer programs to predict scattering from a variety of structured particles. For marine organisms with spherical symmetry, rigorous calculations can be performed for unrestricted size and optical properties using Mie theory. Models based on Rayleigh-Debye theory are valid only for a restricted range of sizes and optical properties but predict scattering for a variety of shapes. Computer programs were developed to determine the range of validity of the non-rigorous theories by comparison with rigorous theories for spherical geometries.

A new method was developed for measuring the optical properties of single, immobilized marine organisms. Fixed cells[4] of the dinoflagellate *Prorocentrum micans* were immobilized in a transparent silica gel. Because the solvent in the gel dominates the relative refractive index, the residual scattering caused by the gel can be effectively eliminated. The technique provides a convenient method to perform scattering or other optical measurements on immobilized cells without interference of a substrate in a liquid medium.

PLANNED ACCOMPLISHMENTS FOR FY 1988

Measurements of the sickling behavior of HbS will be expanded to determine the kinetics and quantify the differences in density-gradient-separated red cell populations.

Models will be developed comparing the unrestricted Mie calculations and Rayleigh-Debye approximations for the infinite cylinder. Rayleigh-Debye theory will be used to model more-complex-shaped particles. Preliminary measurements of *Prorocentrum Micans* performed this year revealed an unexpectedly strong circular polarization signal. These measurements will be repeated in FY 1988 with improved equipment and in greater detail.

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Solid-State Radiative Heat Pump*

P. Berdahl

The objective of this project is to establish the research basis for the development of a new class of heat pump. This new heat pump will be a solid-state device that accepts input energy in the form of electricity and pumps infrared (heat) radiation across a thermally insulating gap. An important potential application is the heating and cooling of buildings, including applications using thermal storage.

Semiconductor materials with direct narrow bandgaps in the range of 0.03-0.25 eV emit equilibrium thermal radiation which is in large part due to electron-hole recombination. An excess or deficit of infrared radiation, compared to the thermal equilibrium value, can be produced when the concentrations of electrons and holes are varied from their thermal equilibrium values by electrical means. Two techniques for varying the concentrations of electrons and holes are of special interest here: (1) electrical bias of a p-n junction to produce carrier injection or, for reverse bias, carrier extraction; (2) the magneto-concentration effect in which orthogonal electric and magnetic fields are used to enhance (or deplete) the concentrations of electrons and holes near the semiconductor's surface. The p-n junction technique seems particularly promising for the development of technologically mature devices, while the magneto-concentration effect offers the opportunity for the study of key recombination phenomena in a simpler experimental system.

Recently, the magneto-concentration effect was employed to explicitly demonstrate a galvanomagnetic radiative cooling effect.[1] This experiment proved that working solid-state radiative heat pumps can be constructed. However, increases in efficiency are required for this technology to compete with more conventional heating and cooling techniques.

ACCOMPLISHMENTS DURING FY 1987

Ongoing measurements of the quantum efficiency of radiative recombination in InSb were continued in order to clarify the values that this key sub-efficiency can take and to determine whether or not this efficiency can be improved by doping, as suggested by theoretical considerations. Figure 1

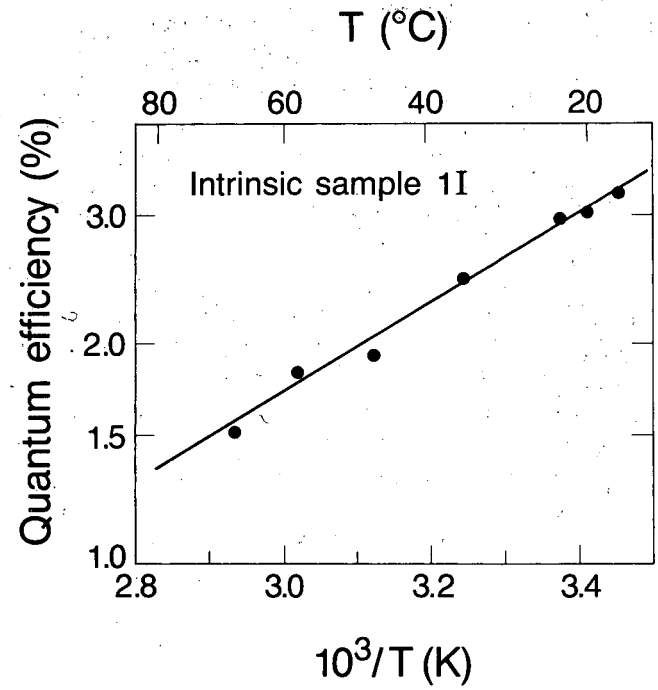

Figure 1. Measured quantum efficiency of radiative recombination (logarithmic scale), in a pure sample of InSb, as a function of temperature. The solid line is a fit to the data. (XBL 873-6243)

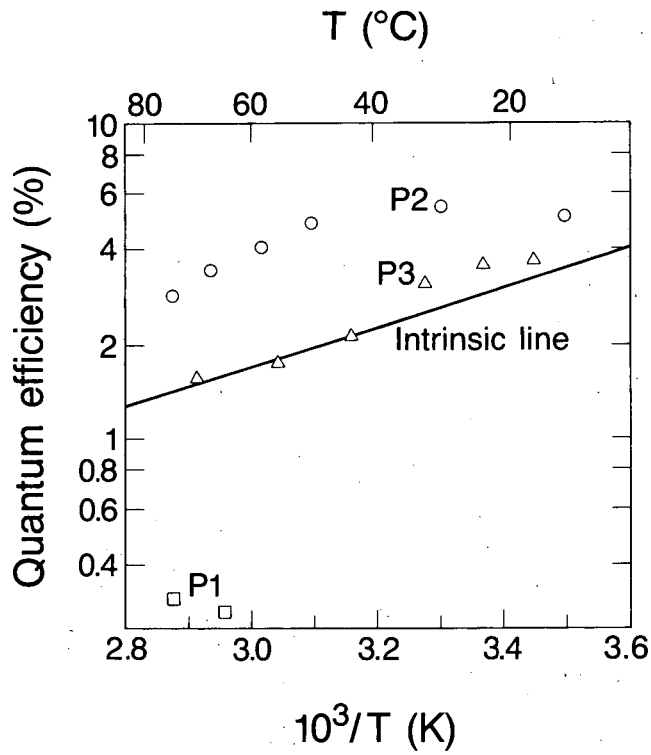

Figure 2. Measured quantum efficiencies for radiative recombination. The solid line is from Fig. 1. The doping (impurity) concentration, in units of 10^{16} cm^{-3}, is 4.2 for sample P3, 25 for sample P2, and 140 for sample P1. (XBL 873-6246)

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shows measured values of the quantum efficiency of radiative recombination in pure (intrinsic) InSb as a function of temperature, as measured using our galvanomagnetic luminescence technique.[2] The efficiency is 3% at room temperature, too low to form the basis of a highly efficient heat pump. However, Fig. 2 shows that the addition of p-type impurities (cadmium atoms in this case) can raise the quantum efficiency to values at least as high as 5%. The detailed interpretation of these results [3] is that p-type impurity atoms suppress the dominant form of non-radiative recombination (the Auger mechanism), and therefore enhance the importance of radiative processes. The Cd impurities also introduce new non-radiative recombination processes, so there is an optimum level of doping, with an impurity concentration of roughly 2×10^{17} atoms cm^{-3}.

PLANNED ACTIVITIES FOR FY 1988

Further research on InSb is desired and may be expected to raise the quantum efficiency for radiative recombination even further. However, it is important to begin the evaluation of other promising narrow-bandgap semiconductor materials, such as the lead-tin-tellurides, to determine their suitability for applications in solid-state radiative heat pumps. Therefore future research will include studies of radiative recombination with these unexplored materials.

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Processing of Condensate Waters from Coal Gasification*

C.J. King, J. Senetar, T. Grant, L. Poole, and R. Thompson

Condensate waters from low-temperature coal-gasification processes contain large concentrations of ammonia, acid gases, and dissolved organics – notably phenolic compounds. For both economic and environmental reasons it is necessary to purify these waters sufficiently to allow recycle, probably as make-up to a cooling-tower system. The principal objective of this project has been to provide basic understanding enabling improved solvent-extraction, adsorption, and stripping processes for these condensate waters. Current research focuses upon removal of organics by regenerated carbon adsorption processes, and development of a more energy-efficient approach for recovery of ammonia.

Use of carbon adsorption for condensate waters is held back by incomplete regeneration of the carbon, which typically requires replenishment of 15% or more of the carbon per cycle. Our goal is to identify the cause of this irreversibility and to develop means of overcoming or lessening the problem.

Stripping of ammonia from condensate waters is energy-intensive, because the volatility of ammonia is lowered by the presence of dissolved acids, notably carbon dioxide and hydrogen sulfide. We have pursued an improved approach, wherein ammonia is extracted with a liquid ion exchanger, while the acid gases are simultaneously stripped. This greatly reduces the steam requirement for stripping and serves to isolate ammonia as a product.

ACCOMPLISHMENTS DURING FY 1987

Adsorption of Phenols

Through several complementary experimental approaches we have confirmed that phenols undergo a slow chemical reaction with carbon surfaces. The reaction is apparently irreversible, leading to higher molecular-weight products, which we have been able to identify by liquid chromatography of leachates. Solvent regeneration by liquid extraction is more efficient than regeneration by heating and vaporization. Several common solvents give nearly complete recovery of unreacted adsorbed phenols.

Isolation and Recovery of Ammonia

We have shown that organophosphinic acids have optimum basicity for extracting ammonia from condensate waters (favored by high basicity) with efficient regeneration by distillation of ammonia (favored by low basicity). We have developed a means of purifying Cyanex 272, a commercial phosphinic acid extractant, and have used the purified extractant to determine and interpret extraction equilibria and regenerability.

PLANNED ACTIVITIES FOR FY 1988

Adsorption of Phenols by Carbon

We are observing reaction kinetics for different phenolic solutes as they react with carbons having different surface characteristics, so as to define the chemistry of the reaction between phenols and carbons. This information is used to identify processing approaches which minimize irreversibility and hence minimize carbon consumption.

Extraction of Ammonia

We are carrying out experiments with purified Cyanex 272 to characterize the amount of increased aqueous solubility and/or increased vapor pressure of hydrocarbon decomposition products resulting from heating during distillation. Since process efficiency is increased by carrying out the distillation of ammonia from the extractant at higher temperatures, the temperature limit for thermal degradation determines the overall efficiency of the extractive approach for ammonia recovery.

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Removal of H_2S from Coal-Derived Gases*

S. Lynn, R. Hix, D. Neumann, S. Sciamanna, and C. Stevens

When coal is gasified most of the sulfur is converted to H_2S and must be removed before the gas can be used either as a fuel or as synthesis gas. The UCB Sulfur Recovery Process (UCBSRP) is being developed as a general method for removing H_2S from gases. The H_2S is absorbed in a polyglycol ether, then reacted in the liquid phase with SO_2 to form marketable elemental sulfur and water. The process allows high specificity and flexibility; H_2S can be reduced to the part-per-million level or below in the presence of CO_2 and the other components of gasified coal. The CO_2 may be left in the original gas stream or it may be co-absorbed and recovered as a separate, sulfur-free product. The process thus has application both to syngas and hydrogen production from O_2-blown gasifiers and to power production using an air-blown gasifier.

ACCOMPLISHMENTS DURING FY 1987

Process Configuration Studies

Figure 1 shows a flowsheet for the UCBSRP in a configuration that gives maximum selectivity for H_2S removal. In the primary absorber H_2S is removed principally by physical absorption. The stream of solvent leaving the absorber is nearly saturated with all of the components of the gas being treated. A water wash at the top of the primary absorber prevents loss of solvent vapor in the treated gas.

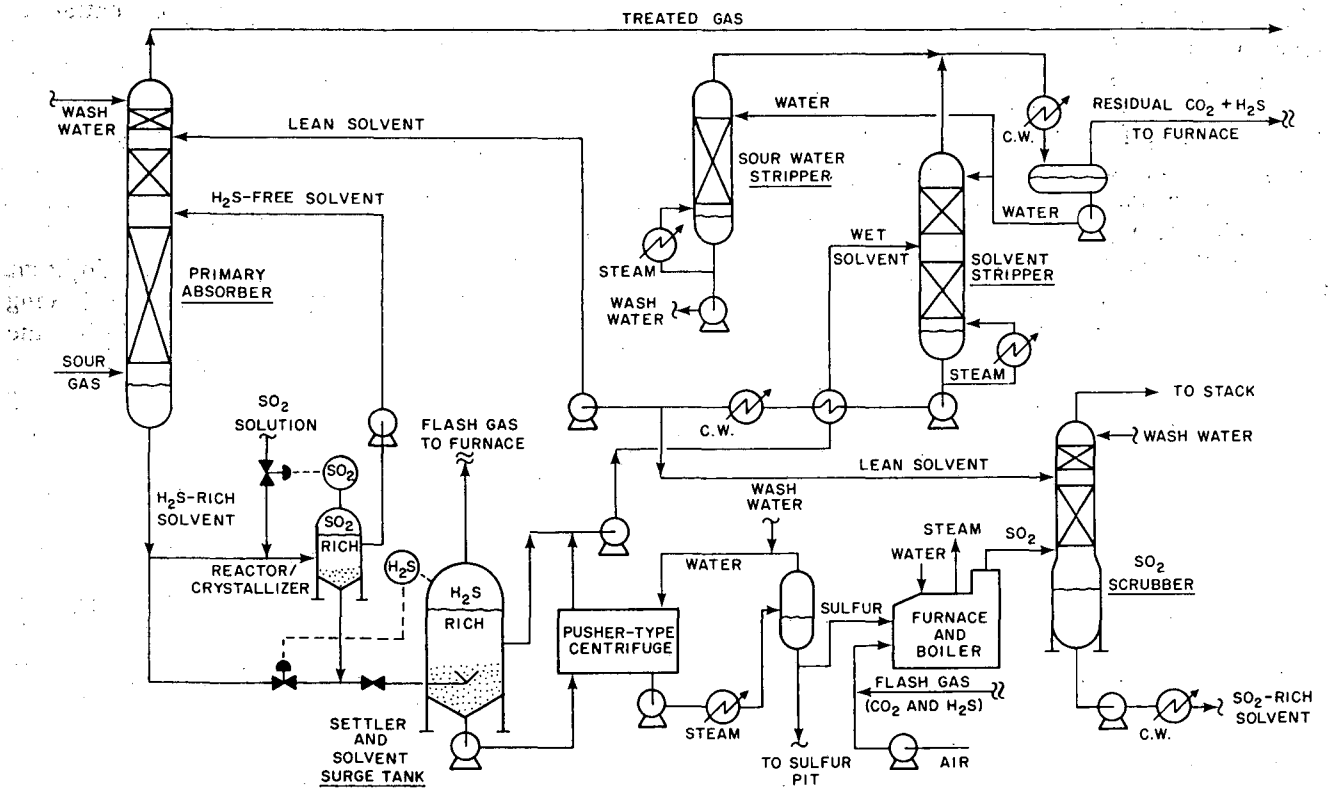

Figure 1. UCB Sulfur Recovery Process–process configuration for high H_2S selectivity. (XBL 882-583)

*This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal Utilization, Division of Surface Coal Gasification of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Most of the solvent stream leaving the primary absorber then enters a reactor/crystallizer that operates at the pressure of the primary absorber. A second solvent stream containing SO_2 is metered into the same reactor at a rate that keeps the SO_2 content within the reactor a few percent above stoichiometric relative to the H_2S. (It is necessary to have an excess of one reactant or the other in each reactor to avoid excessive reactor volumes and the need for highly precise reactor control). A clarified overflow from the SO_2-rich reactor is pumped back to the primary absorber. This solvent stream has been completely freed of its H_2S content but is still saturated with respect to the other components in the gas being treated in the primary absorber. The net co-absorption of these other gas components (such as CO_2) is thus kept quite small and the effective selectivity for H_2S is of the order of 50 to 100. The SO_2 content of this solvent stream, although low, provides a chemical enhancement for the absorption of the H_2S on the upper trays of the primary absorber to facilitate meeting very stringent H_2S specifications in the treated gas. (The temperature in the primary absorber is high enough to prevent precipitation of the sulfur formed by this reaction. Not shown in Fig. 1, to avoid clutter, is provision for cooling both reactor/crystallizers with cooling water so that the solvent is sub-saturated in sulfur at all other points in the system).

The underflow from the SO_2-rich reactor carries the sulfur and water formed in the reaction between H_2S and SO_2. The flow of this stream is sized to keep the water content of the solvent from exceeding 5% and is directly proportional to the rate of H_2S removal – the flow will typically be about 10% of the total flow of solvent through the primary absorber. Sufficient H_2S-rich solvent, from the primary absorber, is added to the stream to leave a small excess of H_2S after all of the residual SO_2 has reacted. This stream is then flashed to atmospheric pressure in the settler/surge tank.

The sulfur made in the process forms a slurry in the underflow from the surge tank. The sulfur is recovered and washed in a centrifuge. In most cases about one-third of the sulfur will be burned in the furnace to make the SO_2 needed in the process. The energy recovered in the waste-heat boiler will usually supply and perhaps exceed the energy required by the process.

The overflow streams from the surge tank and the centrifuge are combined and sent to the solvent stripper. Boiling most of the water out of the solvent provides a stripping vapor that also removes unreacted H_2S and co-absorbed gases such as CO_2 from the solvent. Most of the solvent leaving the solvent stripper is used in the SO_2 scrubber where it absorbs the SO_2 from the combustion gas leaving the furnace. The SO_2 content of this solvent is nil, and hence the SO_2 content of the stack gas leaving the scrubber can readily be reduced to the part-per-million level. The remainder of the solvent from the stripper is sent to the primary absorber, where it prevents loss of SO_2 in the treated gas.

Figure 2 shows a process configuration suitable for removing and recovering one or more components (in addition to the H_2S) from the gas being treated, such as removing CO_2 from a synthesis gas ahead of a shift reactor in a process for producing hydrogen. The operation of this process is identical to that described above in many respects. It differs as follows: the H_2 and CO are stripped from the solvent. The stripping gas is obtained by a partial flash of the solvent immediately downstream of the primary absorber. Most of the H_2S-rich solvent stream leaving the flash drum, together with a controlled flow of SO_2 solution, enters an SO_2-rich reactor. The pressure of the SO_2-rich solvent stream is reduced in stages (only two are shown) to about one atmosphere. The off-gas from each stage is recompressed to the pressure desired for the CO_2 product and is contacted with neat solvent to remove traces of SO_2, then washed with water to recover solvent vapor. For the case shown, in which a high degree of CO_2 removal is not required, clarified H_2S-free solvent from the atmospheric flash can be pumped directly back to the primary absorber.

As in the flow configuration designed for high H_2S selectivity, the sulfur and water formed in the reaction are conveyed out of the last SO_2-rich reactor in a stream that is rendered H_2S-rich with by-passed H_2S solution. As before, the flow of this stream is proportional to the rate of sulfur production.

Corrosion Studies

Corrosion studies were performed by submerging metal coupons half way in a solution of H_2S or SO_2 in a glycol ether. To make the system as corrosive as possible, the solvent was a mono-ether (which is also an alcohol) and sulfur and water were added in concentrations twice (or greater) those encountered in the process. The exposure was carried out for three successive 20- to 30-day periods at each temperature. Table 1 shows the corrosion rates observed. Since 60°C is the maximum temperature at which SO_2 is present (outlet of the SO_2 absorber), carbon steel and 304 and 316 stainless steels should corrode at rates much less than 1 mil/year (0.02 mm/yr) under all process conditions.

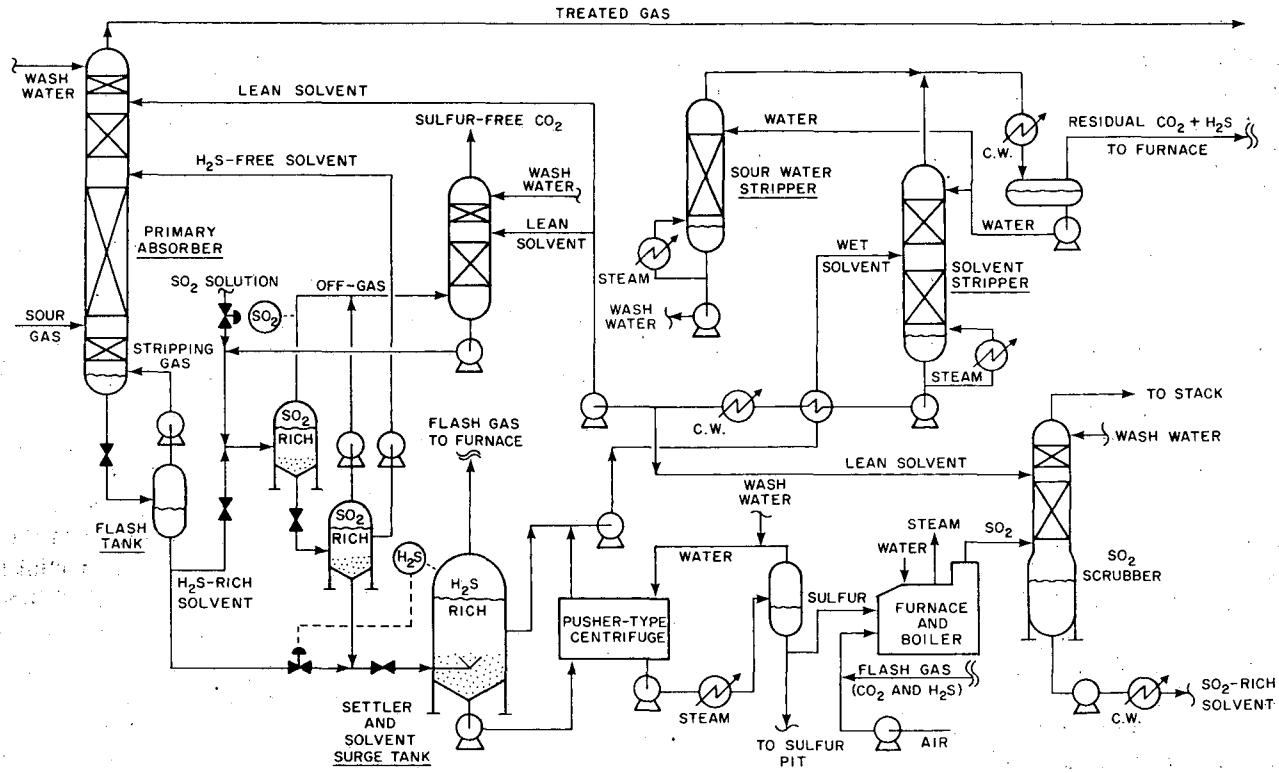

Figure 2. UCB Sulfur Recovery Process–process configuration for co-absorption of CO_2. (XBL 882-582)

Sulfur Crystallization

A major potential advantage of the UCB Sulfur Recovery Process is the purity of the crystalline sulfur that is produced. The sulfur crystallizes from solution both as a result of cooling and as a result of chemical reaction between H_2S and SO_2. In the former case the degree of supersaturation is relatively low because the solubility of sulfur in the solvent varies only a few grams per liter over the temperature range of interest. A substantially higher concentration of sulfur can result from the chemical reaction.

The crystallizer consists of a well-stirred 2-liter vessel. Hot saturated feed enters at the top, and the vessel walls are cooled. Cold effluent exits at the bottom of the vessel as a sulfur/solvent slurry. A sample of the effluent slurry is collected when the system is at steady-state and the size distribution of the sulfur crystals is determined.

Table 1. Corrosion Rates of Steels in Process Solutions.

	MEASURED RATES AND CONDITIONS *		
Metal	SO_2: @ 100°C	@ 120°C	H_2S: @ 150°C
Carbon Steel	0.6	1.7	0.05
304 Stainless	0.7	1.5	0.02
316 Stainless	1.3	4.8	0.01

* Mils/year in diethylene glycol methyl ether, 5% H_2O, saturated with sulfur, 50 - 100 psi gas pressure.

Gas Absorption with Chemical Reaction

Tray efficiency data are needed for two process situations. In one, H_2S at very low concentration is being absorbed by a chemically reactive solution of SO_2. In the other, gaseous SO_2 in the low parts-per-million concentration range is absorbed by lean process solvent. Both are of interest because one wishes to effect very stringent sulfur removal with the UCBSRP. The equipment consists of a single sieve tray (or section of packed column) placed in a test section through which gas and liquid streams pass. Murphree tray efficiencies are determined from the mass balances and previously obtained solubility data.

PLANNED ACTIVITIES FOR FY 1988

The crystallizer is being modified to incorporate crystal size classification to retain smaller crystals and produce a product of larger size. Sulfur will be produced by chemical reaction. Data obtained for absorption of H_2S enhanced by the presence of SO_2 in the solvent will be used to develop a model that incorporates the reaction kinetics work done previously.

A computer model that simulates all of the unit operations in the process is operational and facilitates process synthesis for specific applications. It will be used to evaluate and further refine the process configurations shown in Figs. 1 and 2 for the purification of hydrogen derived from gasified coal.

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Analysis of Coal Gasification Reactors*

M.M. Denn and G. Dow

This research project is concerned with modeling moving-bed coal gasifiers in order to gain insight into reactor operability and design. Detailed single-particle models seem to provide the most realistic description of the transport phenomena and chemical kinetics near the coal surface. Rather than modeling the complete reactor as a continuum of individual particles, we describe the flow pathway of the gases through the coal bed as a plane channel whose sides are composed of reactive carbon. This pore model of the gasifier incorporates a detailed description of the coal surface which implicitly accounts for particle-particle interactions.

ACCOMPLISHMENTS DURING FY 1987

An automatic remeshing scheme has been incorporated into our numerical method for solving the model equations. With a fixed number of nodes, this scheme adjusts the finite-difference mesh so that the nodes are concentrated in the region where rapid combustion of carbon generates steep temperature and composition gradients.

We have adapted our model to study the influence of gas-phase oxidation, solid-gas temperature differences, and transverse gradients on predictions of reactor performance. The consideration of these factors as well as the description of the coal surface serves to categorize current modeling efforts.[1]

Figure 1 shows the gas temperature profiles predicted for typical operating conditions in an air-blown Lurgi gasifier. The inclusion of differing solid and gas temperatures lowers the peak temperature and pushes the hot spot closer to the gas feed.

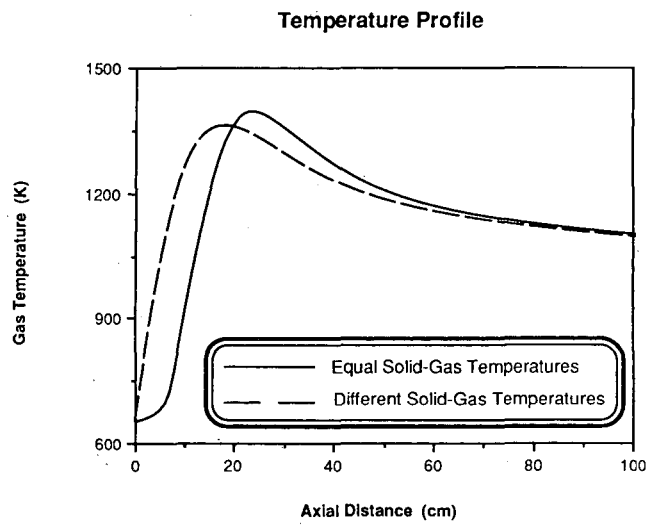

Figure 1. Gas temperature profiles for a one-dimensional channel model of a moving-bed gasifier. (XBL 882-575)

*This work was supported by the Morgantown Energy Technology Center, Assistant Secretary for Fossil Energy, Office of Coal Utilization, Advanced Research and Technology Development, Division of Surface Coal Gasification through the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

PLANNED ACTIVITIES FOR FY 1988

The study will be completed in FY88. We will explore how operating conditions such as blast temperature and reactant feed rates affect reactor performance.

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Energy-Related Organometallic Chemistry*

The work in this area is described in the following four sections.

BIOMIMETIC ORGANOMETALLIC CHEMISTRY

R.H. Fish and R.T. Price

The recent interest in the synthesis of biomimetic catalysts that mimic the biologically important cytochrome P-450 dependent monooxygenase enzyme reaction[1-3] by converting C-H bonds to C-OH bonds in a regio- and stereoselective manner has led to an enormous number of contributions that have clearly shown similar reactivity to the reactive metal center of that enzyme.[4-6] While the types of substrates that have been studied with these biomimics have included alkanes and alkenes, it was surprising, therefore, to discover that no examples of organometallic substrates have been reported with these biomimetic catalysts.

One class of organometallic compounds, the organotins, have been shown to have a wide variety of biological activity[7] and have been studied in depth with a cytochrome P-450 enzyme system from rat liver microsomes.[8-13] Those studies were unequivocal in determining that the tin atom controlled the regiochemistry when substrate steric effects at the binding site in proximity to the active metal center were not a factor.[8,9] In addition, those studies clearly were among the first to assign a free radical mechanism to the P-450 enzyme in the conversion of C-H bonds to C-OH bonds, with the tin atom able to stabilize the intermediate carbon radicals that were alpha and beta to it.[8-11,14]

More importantly, we were also able to study, with the enzyme system, the regio- and stereoselective aspects of this conversion with cyclohexyltriphenyltin, **1**, and demonstrate that steric effects at the binding site in proximity to the active metal center control the regiochemistry. Thus, we have reported the first example of the use of an organometallic substrate, **1**, with "oxo" metalloporphyrins that have been shown to be biomimetic catalysts for the cytochrome P-450 active metal center, iron(III) or manganese(III) tetrakis(pentafluorophenyl)porphyrin derivatives $[TPF_5P(Br,OAc)]^5$ in the presence of the oxygen transfer agent, iodosylbenzene, and establish the regio- and stereoselectivity of the hydroxylation reaction, while comparing the results to those found for the enzyme system.

Accomplishments During FY87

The regio- and stereoselectivity in the hydroxylation reaction of cyclohexyltriphenyltin with biomimetic catalysts that mimic the important cytochrome P-450 monooxygenase enzymes, the iron(III) and manganese(III) tetrakis(pentafluorophenyl) porphyrin derivatives, was studied with the oxygen transfer agent, iodosylbenzene, and the results compared to those obtained for the enzyme. It was found that the regioselectivity on a per hydrogen basis for the biomimetic catalysts provided a C4:C3:C2:C1 ratio of 1:2:6:0 and a high stereoselectivity of equatorial to axial hydroxyl products, with a EQ/AX ratio of 29. The enzyme had a regioselectivity ratio with C4:C3:C2:C1 being 109:7:1:0 and a high EQ/AX ratio of 59. The dramatic regiochemical differences between the biomimic and the cytochrome P-450 monooxygenase enzyme can be explained by the fact that the enzyme provides steric constraints at the binding site in proximity to the active oxo metal center, while the biomimics we utilized did not have these constraints. The hydroxylation results with the biomimetic catalysts also suggests a free radical reaction, since the carbon-tin bond can stabilize intermediate carbon radicals and gave *trans*-2-hydroxycyclohexyltriphenyltin and *cis*-3-hydroxycyclohexyltriphenyltin as the major oxidation products. They also suggest a free radical cage effect, since we observed a high EQ/AX ratio and the absence of *cis*-2 and *cis*-4-hydroxycyclohexyltriphenyltin products.

Planned Activities for FY88

We plan to concentrate on the C-H activation of hydrocarbons with biomimetic catalysts.

*This work was supported by the Electric Power Research Institute; the Assistant Secretary for Fossil Energy, Office of Oil, Gas and Shale Technology, through the Bartlesville Project Office; and the Director, Office of Energy Research, Office of Basic Energy Science, Chemical Sciences Division, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

BIOMIMETIC CARBON-HYDROGEN ACTIVATION CHEMISTRY

R.H. Fish, R.T. Price, and R.H. Fong

The use of biomimetic catalysts that convert C-H bonds to C-OH bonds in the presence of an oxygen source is an area of intense research interest.[4-6] The enzyme that has been most important in the success of these biomimetic studies has been cytochrome P-450, which has been studied in-depth.[1-3] Recent findings have clearly shown that shape selectivity, built into the biomimics at the active metal center, is an important parameter for comparison of the regiochemical results of the mimics to those obtained with the P-450 enzyme.

More-recent reports have focused on supramolecule porphyrins[15-19] that contain a microenvironment more representative of the enzymes and these have been shown to be able to bind oxygen,[15] oxygenate olefins[19] and do C-H activation chemistry[20] with a monooxygen reagent. We were intrigued by the possibility that the supramolecule porphyrins would show any special reactivity in the carbon-hydrogen activation of their putative intermediate "oxo" derivatives with small hydrocarbons (C_1-C_3) to preferentially form the corresponding alcohols from those hydrocarbons. To our knowledge, this is the first reported attempt of C-H activation chemistry with C_1-C_3 hydrocarbons with a supramolecule metal porphyrin catalyst and allows an evaluation of the microenvironment surrounding the active metal center compared to an open-face porphyrin as well as kinetic and thermodynamic factors that control C-H activation.

Accomplishments During FY87

The manganese (III) complex of the doubly looped, superstructured amide ligand, **1**,[18] was evaluated in the C-H activation reactions of methane, ethane, propane and cyclohexane to provide the corresponding alcohols using iodosylbenzene as the monooxygen transfer agent. Table 1 compares the results using catalysts **1** and **2**, an open-face, meso-substituted manganese porphyrin, Mn(III)TF_5PP(OAc), to provide information on the C-H bond reactivity of the four hydrocarbons studied. This includes the yield of the product alcohol, ketone or chloride and the turnover number.

Planned Activities for FY88

Since our goal is C-H activation of methane and ethane to their respective alcohols, we are presently evaluating biomimetic porphyrin and non-porphyrin

Table 1: Carbon-Hydrogen Activation of Hydrocarbons Using Compounds **1** and **2** as Catalysts and Iodosylbenzene as the Monooxygen Transfer Agent.[a]

Hydrocarbon	Product (%)[b]		Turnover No.	
	1	2	1	2
CH_4	NPD[c]	NPD		
CH_3CH_3	CH_3CH_2OH (1)	CH_3CH_2OH (2.7)	0.23	0.54
$CH_3CH_2CH_3$	$(CH_3)_2CHOH$ (9.6)[d]	$(CH_3)_2CHOH$ (13.5)[e]	2.1	2.8
	$CH_3CH_2CH_2OH$ (0.6)	$CH_3CH_2CH_2OH$ (1)		
CycloC_6H_{12}	$C_6H_{11}OH$ (72)	$C_6H_{11}OH$ (69.4)	16.7	14.0
	$C_6H_{10}O$ (5.2)	$C_6H_{10}O$ (1)		
	$C_6H_{11}Cl$ (4.5)	NPD		

[a]Reactions of methane, ethane and propane were run in a Parr kinetic apparatus at room temperature for 24 h at 100-500 psi with a iodosylbenzene to catalyst ratio of 20:1. Catalyst concentration was at room temperature in Schlenk tubes with substrate: iodosylbenzene: catalyst ratios of 1100:20:1 in methylene chloride. Analysis and quantitation of products was obtained via capillary column GC analysis with a 15m • .035 mm DB5 column.
[b]Based on the mmoles of iodosylbenzene.
[c]No product detected.
[d]Ratio of 2° to 1° C-H bond reactivity on a per H basis is 45:1.
[e]Ratio is 42:1.

catalysts that have longer half-lives and better shape selectivity to overcome the thermodynamic disadvantage of an appreciable C-H bond dissociation energy and to hopefully provide a kinetic advantage for activation.

POLYMER PENDANT LIGAND CHEMISTRY, 2

R.H. Fish, A.D. Thormodsen, R.B. Belser, Jr., G. Friedman and J.G. Reynolds

The use of polymer pendant ligands to remove metal ions from solution is an area of intense research interest. The applications for facile metal ion removal with these pendant ligands are unlimited; however, in most of the reported applications the molecular structures of the metal compounds, both in the complex media in which they are present and those that are formed on the modified polymers, are not always clearly defined.

Thus, in this paper,[21] we report studies on the reactions of both 2% and 20% CAT-PS-DVB resins with $VO(AcAc)_2$ at various times and at equilibrium, as well as the diffusion limitations of increased cross-linking, and the effects of the base, triethylamine, and the bidentate ligand, bipyridine, on the equilibrium value for removal of vanadyl ion from solution. We have also addressed the structure of the vanadium complexes on the 20% CAT-PS-DVB resin by infrared and EPR spectroscopic techniques. As well, vanadium distributions for both the 2% and 20% CAT-PS-DVB resins were determined by SEM and EDX analysis.

Accomplishments During FY87

The reactions of catechol ligands, bonded to either 2% or 20% cross-linked methylated polystyrene-divinylbenzene resins, (CAT-PS-DVB), with vanadyl acetylacetonate [$VO(AcAc)_2$] were studied. Vanadyl ion removal from solution at equilibrium was 0.104 mmol V/g of resin and 0.075 mmol V/g resin for the 2% and 20% CAT-PS-DVB resins, respectively. It was found that the 20% cross-linked modified resin was limited in the vanadyl ion ligand-exchange reaction by diffusion into the resin, while this was not the case for the 2% cross-linked modified resin. The effect of the base, triethylamine, dramatically increased the amount of vanadyl ion removed from solution, via ligand-exchange, and was thought to occur by deprotonation of the catechol ligand. The bidentate ligand, bipyridine, had no effect on the removal of vanadyl ion in the ligand-exchange reaction and thus apparently does not form a 1:1 complex with the vanadium catecholate bonded complex. The structures of the vanadium catecholates on the resin were tentatively established by infrared and electron paramagnetic resonance (EPR) spectroscopy to include two vanadium (4+) complexes–a vanadyl bis(catecholate) complex, $[\bigcirc-VO(CAT)_2]^{2-}$, and a distorted tris(catecholate) complex of octahedral geometry, $[\bigcirc-V(CAT)_3]^{2-}$. Scanning electron microscopy (SEM) and energy dispersive analysis (EDX) studies were also performed on the 2% and 20% cross-linked vanadium-containing CAT-PS-DVB resins to clearly show a uniform distribution of vanadium throughout both the resins.

Planned Activities for FY88

We plan to publish a complimentary study on polymer-pendant nickel catecholates.

STUDIES ON THE BONDING OF POLYNUCLEAR HETEROAROMATIC NITROGEN COMPOUNDS TO PENTAMETHYLCYCLOPENTADIENYL-RHODIUM DICATION: NITROGEN VERSUS π-COMPLEXATION

R.H. Fish and H-S. Kim

In recent studies on the regioselective hydrogenation of polynuclear heteroaromatic nitrogen compounds with mononuclear rhodium and ruthenium homogeneous catalysts , it was evident that the substrate nitrogen compound was bound to the catalyst metal center prior to hydrogen transfer. This bonding of the nitrogen heterocyclic compound to the metal center was pivotal for the selective hydrogenation of the nitrogen-containing ring. Therefore, in order to determine more unequivocally the nature of this substrate bonding, i.e., nitrogen (N) versus π-bonding, we have initiated studies on the reactions of several representative polynuclear heteroaromatic nitrogen compounds with pentamethylcyclopentadienylrhodium dication, [Cp^*Rh^{2+}].

The previous limited studies with Cp^*Rh^{2+}. and nitrogen compounds showed π bonding with indole (benzene ring) and, to our knowledge, no other complexes with polynuclear heteroaromatic nitrogen ligands and Cp^*Rh^{2+} have been reported. Thus, we report preliminary findings that dramatically show that the structure of the nitrogen ligand and availability of nonbonding electrons on the nitrogen atom determines N versus π-bonding to Cp^*Rh^{2+}.

Accomplishments During FY87

The general synthetic reaction procedure which we followed is shown in Eq 1:

$$[Cp^*RhCl_2]_2 + AgX \xrightarrow{\text{acetone}} [Cp^*Rh(acetone)_3]^{2+}\,X_2$$

$$(X = BF_4 \text{ or } PF_6) \qquad \downarrow \text{"N"}$$

$$[Cp^*RhN_{1\text{ or }3}]^{2+}\,X_2$$

"N" = compounds **1–5**

The reactions of quinoline, **1**; 1,2,3,4-tetrahydroquinoline, **2**; 2-methylquinoline, **3**; N-methylindole, **4**; and N-methylpyrrole, **5**, with pentamethylcyclopentadienylrhodium dication $[Cp^*Rh(Acetone)_3^{2+}X_2$, PF_6 or $BF_4]$ were studied to ascertain nitrogen (N) versus π-bonding. Ligands **2**, **3**, **4** and **5** preferred η^6 coordination, while **1** was found to form a tris nitrogen bonded complex.[22]

Planned Activities for FY88

We are presently further evaluating Cp^*Rh^{2+} as a hydrogenation catalyst for polynuclear heteroaromatic nitrogen compounds; obtaining single crystal X-ray analyses for all rhodium complexes; studying the reactions of the rhodium complexes with hydrogen gas and hydride ion; and also studying the bonding of ligands **1-5** with cyclopenadienylruthenium cation.

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Ammonia Removal from Oil Shale Process Waters Using Tubular, Microporous Polytetrafluoroethene Membranes*

R.H. Sakaji, C.G. Daughton, R.E. Selleck, and J.F. Thomas

Ammoniac industrial and domestic wastewaters contain both dissolved ammonia gas (NH_3, a base) and nonvolatile, protonated ammonium ion (NH_4^+, the conjugate acid). The relative concentrations of these two species depends on the pH (pK_a = 9.3 for NH_4^+ at 30°C). The concentration of ammoniac-nitrogen reported for a wastewater does not distinguish between the two forms, and it can range over orders of magnitude: domestic sewage (typically 10 to 50 mg/L),[1] oil refinery wastewaters (as high as 7,000 mg/L),[2] and oil shale process waters (1,000 to 31,000 mg/L).[3]

Ammonia removal from refinery wastewaters typically depends on a packed-bed process, such as energy-intensive steam-stripping. Studies by the American Petroleum Institute have shown that steam stripping is not always effective.[4] Since alternative technologies would be desirable, this project has investigated gas-permeable membrane separation, specifically nonosmotic dissolved-gas dialysis (NOGD), as an alternative to conventional steam stripping.[5] Using NOGD, ammonia diffuses from the wastewater (a region of high concentration) to a dialysate fluid (a region of low concentration) without the concomitant osmosis of liquid water. The semi-permeable separation device comprises tubular polytetrafluoroethene (PTFE) membranes, which combine hydrophobic and microporous properties to allow gases to volatilize from a liquid and diffuse through the gas-filled membrane pores while preventing the passage of liquid water. The wastewater is thereby not diluted by osmosis, and highly concentrated dialysates can be produced. The transport of ammonia is driven by a concentration gradient maintained across the membrane by absorption of the ammonia-gas permeate into a dilute, nonvolatile acid solution, where it is protonated to form ammonium ion. This effectively reduces the ammonia concentration at the outer membrane wall to zero. NOGD would not only be less energy intensive and more selective, it would also succeed in combining stripping and resource recovery into a single unit process; this simplifies design and encourages recovery of a potentially valuable resource (ammonia for fertilizer).

*This work was supported by the Assistant Secretary for Fossil Energy, Office of Oil, Gas, and Shale Technology of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, through the Bartlesville Project Office, Bartlesville, OK.

ACCOMPLISHMENTS DURING FY 1987

The subject of the work summarized here is a numeric model for the mass transfer of ammonia, with the objective of understanding how ammonia is transported through the PTFE membranes. A detailed numeric model was built from the equation of continuity; effects such as dispersion and diffusion were modeled as separate phenomena. The NOGD process was modeled assuming the wastewater to be an incompressible fluid that is pumped through a tubular membrane with steady laminar flow in a direction, z, parallel to the membrane wall. The velocity profile is fully established and is parabolic. Ammonia is transported only by diffusion in the radial direction and by convection in the z-direction (diffusion in the z-direction is negligible in comparison). The model further assumes that there is no chemical reaction that consumes or produces ammonia while the wastewater is in the PTFE membrane. The equations and method of solution for the set of equations are identical to the "extended Graetz" problem,[6] which can be solved by using the separation-of-variables technique. The accuracy of the computer program used to solve this system was verified and shown to be accurate to four significant figures.[7]

The model was used to calculate average ammonia concentrations in the PTFE reactor effluent, and these were compared with experimental results. A disadvantage in this approach is that changes in the average ammonia concentration θ (the ratio of effluent concentration to influent concentration) over a range of dimensionless residence times γ does not follow a simple proportionality. It was therefore necessary to transform and normalize the data so that changes in θ with respect to γ did not affect the comparison of experimental and predicted data. This was accomplished by determining mass-transfer coefficients, k_{expt} and k_{calc}, from the experimental and predicted average concentrations, respectively.[7]

The numeric model was tested using the experimental results from an isothermal, countercurrent NOGD reactor comprising three concentric tubes: an inner, PTFE tubular membrane, a middle glass tube containing the acid dialysate (sulfuric acid, 1.0 N, was selected as the dialysate acid because it is nonvolatile), and an outer glass tube that served as a

temperature-controlled jacket. The tubular PTFE membranes were manufactured by W.L. Gore and Associates, Inc. (Elkton, MD) (i.d. = 1.0 mm; o.d. = 1.8 mm; maximum pore size = 2.0 μm; porosity = 0.50).

The NOGD reactor was used to treat ammonium hydroxide solutions (700-800 mg-N/L), three oil shale process waters (1,130-24,700 mg-N/L), and a sample of domestic sewage. Samples from the ammonium hydroxide experiments were immediately analyzed for total-N by the rapid method of combustion/chemiluminescence (C/CL).[8] These values were equivalent to ammoniac-N since ammonia was the only nitrogenous compound present. The wastewaters were analyzed for ammonia by the phenate colorimetric method.[3] Composite samples of the effluents were collected after the NOGD reactor reached steady-state operation (more than 100 reactor volumes). Since dissolved ammonia gas rather than ammonium ion was the species of interest, ammonia concentrations were calculated from the sample pH using the pK_a of ammonium ion.

The relationship between the experimental results and predicted values were demonstrated by plotting the experimental versus predicted fraction of ammonia remaining. A perfect correlation would yield a line with a slope of unity and a zero intercept (broken line, Fig. 1). Since the ideal line was within the 95% confidence limits of the regression line for the ammonium hydroxide solution, the difference between the experimental and predicted results was probably not significant. The agreement between predicted values and experimental results indicated that the proposed mechanisms of ammonia transport in the numeric model (i.e., radial diffusion, tortuous gas-phase diffusion through the membrane, and longitudinal convection in laminar flow) accounted for the major transport mechanisms during treatment of an aqueous ammonium hydroxide solution.

Data obtained from the oil shale retort water experiments correlated with predicted values (indicated by regression analysis of the experimental θ against the predicted θ) (Fig. 2). The data deviated significantly (as shown by analysis of variance at 99% confidence level), however, from the ideal correlation (broken line, Fig. 2). The regression lines all lie above the ideal case, an indication that performance was poorer than predicted by the model. The increased resistance to mass transfer possibly resulted from pH-dependent reactions (e.g., production or consumption of ammonia) or physicochemical interactions at the gas-liquid interface (e.g., surfactants, such as fatty acids, which are endogenous to retort waters). Neither of these factors was included in the numeric model.

The ammonia removals from Oxy-6, Paraho, and Geokinetics oil shale process waters (56%, 64%,

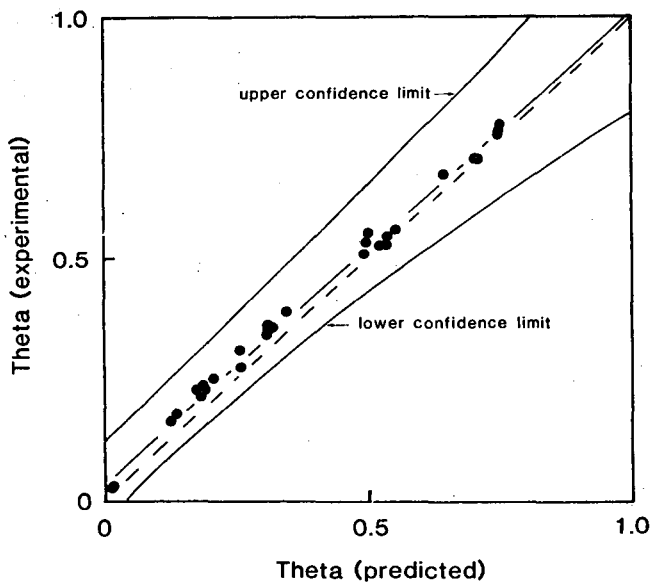

Figure 1. Regression analysis of the experimental fraction remaining (θ) versus the predicted fraction remaining after NOGD treatment of an ammonium hydroxide solution; solid line (least-squares fit), dashed line (ideal fit) with 95% upper and lower confidence limits for the regression line. (XBL 8611-4628)

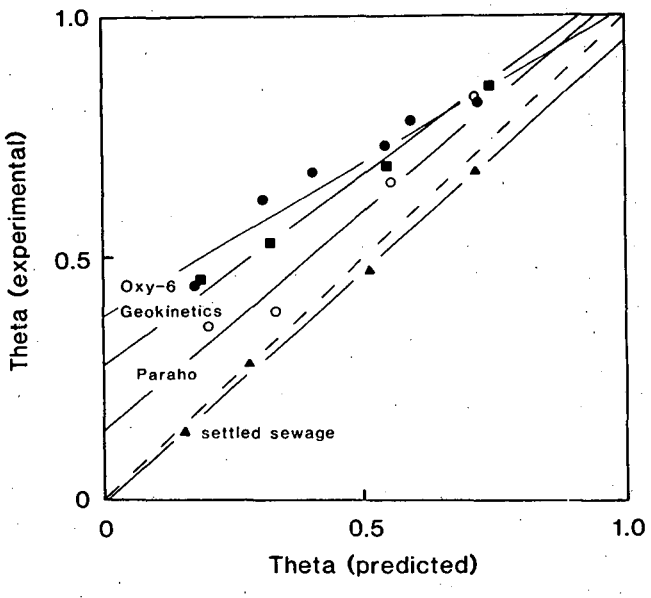

Figure 2. Regression analysis (solid lines) of the experimental fraction remaining (θ) versus the predicted fraction remaining after NOGD treatment of wastewaters: Oxy-6 (solid circles), Geokinetics (solid squares), and Paraho (open circles) oil shale retort waters; domestic wastewater (solid triangles); dashed line (ideal fit). (XBL 8611-4629)

and 55%, respectively) were obtained at hydraulic residence times of 0.92, 0.83, and 0.87 minutes, respectively. These percentage removals are comparable with those of some pilot- and bench-scale steam strippers.[9]

The close correlation between the model and the ammonium hydroxide experimental results suggests that NOGD and the hollow-fiber gas membrane[10] process are identical in principle, even though they differ in operation. In both processes, concentration gradients are associated with the resistance to mass transfer, and because gradients exist only in the water and the membrane, the only resistance to mass transfer would be encountered in those two phases. This in turn means that no resistance to mass transfer exists in the acid dialysate. The NOGD process therefore is not dependent on the flow rate of the dialysate. This is unlike steam stripping, whose physical operation is dependent on the gas-to-liquid (steam-to-wastewater) ratio.

One physical criterion used to compare the relative economies of various stripping devices is the ratio of gas-liquid surface area to empty-bed reactor volume. For a hypothetical NOGD reactor containing 18 tubular membranes packed in a 1.5-cm i.d. dialysate tube, this ratio would be 300 m^2/m^3, which compares favorably with 550 to 820 m^2/m^3 reported for polypropylene hollow-fiber gas membranes[10] and 62 to 980 m^2/m^3 reported for packed-bed reactors.[11]

Since the surface-area-to-volume ratios are within an order of magnitude, the relative differences between the mass-transfer rates will be determined by the mass-transfer coefficients. The mass-transfer rate in the hollow-fiber gas membrane process will be roughly two orders of magnitude below steam stripping or one order of magnitude lower than NOGD. Even though the mass-transfer coefficients for a packed-bed stripper under identical conditions[10] are an order of magnitude better than that found for the NOGD reactor, consideration of NOGD as an alternative to steam stripping should include its lower operating temperature and enhanced resource recovery.

PLANNED ACTIVITIES FOR FY 1988

NOGD has potential as an alternative to steam stripping for removal of ammonia from both domestic and oil shale process wastewaters. The results of numeric modeling imply that it may be possible to improve NOGD process performance by eliminating the reliance on diffusive transport through the use of turbulence promoters. This will be addressed in future experiments. Once the process has been improved, the feasibility of treating other ammoniac wastewaters can be investigated, a more detailed comparison with steam stripping can be made, and a larger-scale reactor can be constructed and tested.

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Kinetics of Gas-Phase Reactions Between Ozone and Selected Nitrogen Heterocycles from Oil Shale Wastes*

E.R. Blatchley III, J.F. Thomas and C.G. Daughton

Removal of dissolved organic carbon, much of it in the form of organonitrogen compounds (ONCs), from oil shale process wastewaters has proved difficult, if not impossible, using conventional (and unconventional) treatment methods.[1-3] Since many of these ONCs are volatile, atmospheric emissions are likely. Release of ONCs to the atmosphere could be important because (1) they are not specifically regulated since there are currently no significant sources of emission, (2) they have displayed acute toxicity and mutagenic potential, and (3) many are malodorous and exhibit low odor thresholds. Once released to the atmosphere, a compound's atmospheric lifetime and fate will be determined by various physical and chemical processes. Physical processes include condensation of vapors to form aerosols, settling of particles to the earth, washout by dissolution in precipitation, and transport of vapors and particles through the atmosphere. Photochemical reactions are the driving force behind most atmospheric chemistry. They are directly responsible for the decay of some atmospheric pollutants and are essential in the generation of reactive intermediates such as ozone and free radicals. The atmospheric chemistry of most organic pollutants is dominated by free-radical reactions.

ACCOMPLISHMENTS DURING FY 1987

The kinetics of reactions between ozone and certain methyl-substituted nitrogen heterocycles (NHCs) were investigated. Ozone-NHC reaction kinetics were determined to allow comparison with kinetics of other important reactions involving NHCs. These comparisons will allow for determination of the dominant path for chemical degradation in the atmosphere, which will in turn allow for prediction of atmospheric chemical lifetimes. The objective was to determine second-order rate constants for reactions between individual NHCs and ozone. Reactions were assumed to be second order overall, first order in each reactant. Decreases in ozone concentration were assumed to result from reaction with the NHC and from "non-reactive" losses (e.g., collision with reactor walls). Under these assumptions, the time-dependent ozone concentration is described by:

$$d[O_3]/dt = -k_w[O_3] - k[O_3][NHC], \qquad (1)$$

where $[O_3]$ and [NHC] are ozone and NHC concentrations, respectively, k_w is a "wall" rate constant, and k is the second-order rate constant. If $[NHC]/[O_3] >> 1$, then [NHC] will remain essentially constant over time, and the reaction can be described using pseudo-first-order kinetics. Under the assumption that [NHC] is a constant, equation (1) can be solved to give the following analytical solution:

$$\ln([O_3]_0/[O_3]_t) = k't \qquad (2)$$

where k′ is a pseudo-first-order rate constant = k_w + k[NHC]. Equation (2) was used as the basis for experimental design.

An apparatus was designed to allow introduction of known quantities of ozone, air, and individual, pure, vapor-phase NHCs to an evacuated reaction chamber. After introduction of reactants, the reaction chamber was pressurized to 760 mm Hg with ultra-zero air, magnetically stirred, and maintained at room temperature; these conditions approximated those of the troposphere on a mild day. The NHC concentration was monitored using a chemiluminescent nitrogen-analyzer and capillary gas chromatography with flame ionization detection, and ozone concentration was monitored with absorbance scans from 350 to 200 nm using a UV-vis scanning spectrophotometer. Chromatographic analysis of the reactor contents, before and after ozone reactions, confirmed that NHC concentrations remained essentially constant.

From equation (2), a plot of $\ln([O_3]_0/[O_3]_t)$ vs. t yields a line through the origin with slope = k′. For each NHC examined, several values of [NHC] were evaluated, and k′ was determined for each. Each NHC seemed to obey pseudo-first-order kinetics, although some deviations were observed. A plot of k′ vs. [NHC] is linear with slope of k and intercept of k_w. Second-order rate constants were determined for each of the NHCs (Table 1). The compounds selected represent a majority of expected gaseous organonitrogen emissions from oil shale development.

Ozone is a strong oxidizing agent. Therefore, the availability of a compound's electrons for reaction will determine its reactivity with ozone. The aromatic character and electronegativity of the

*This work was supported by the Assistant Secretary for Fossil Energy, Office of Oil, Gas, and Shale Technology of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, through the Bartlesville Project Office, Bartlesville, OK.

Table 1. Second-order rate constants and atmospheric lifetimes[a] for reaction of NHCs with O_3.

Compound	k (10^{-19} cm^3/molec-min)	lifetime[b] (years)
pyridine	1.1	14
2-methylpyridine	2.7	5.8
2,6-dimethylpyridine	3.1	5.0
4-methylpyridine	5.9	2.6
3-methylpyridine	6.0	2.6
2,5-dimethylpyridine	23	0.7
benzene[c]	6.0	2.6
pyrrole[d]	9600	14 (hours)

[a]Values of atmospheric lifetime are based on an assumed ozone concentration of 0.05 ppm.

[b]Atmospheric lifetime is defined as the time required to reduce the concentration of a reactant by a factor of "e", where ln(e) = 1.

[c]Data from reference 4.

[d]Data from reference 5.

aromatic nitrogen atom make the NHCs studied (all were six-membered rings) pi-electron deficient (relative to benzene), and hence relatively non-reactive towards ozone. The kinetics determined in these experiments suggest that reactions involving ozone will not be important in reducing the atmospheric lifetime or in determining the fate of these NHCs. Previous experiments have suggested that direct photochemical reactions are also too slow to be of any significance.[6]

We suspect that the most important mode of chemical transformation for these NHCs in the atmosphere will be free-radical reactions; those involving the hydroxyl free radical are likely to dominate. Since free radical reactions also rely on the availability of electrons for reaction, it seems likely that these radical-mediated reactions will also be slow. If so, then the fate of these NHCs in the atmosphere may be determined by physical rather than chemical processes. Compounds with long chemical lifetimes in the atmosphere are significant in that they can be used as tracers of pollution. Since NHCs have such low natural atmospheric abundance, increases in concentration of NHCs downwind from synfuel development sites could possibly be used as indicators of atmospheric pollution.

PLANNED ACTIVITIES FOR FY 1988

Experiments are planned to determine rate coefficients for reactions between NHCs and hydroxyl radical ($OH^{\bullet}$). Previous studies have found hydroxyl radical reactions to dominate the atmospheric chemistry of many organic compounds. The reactions involving NHCs and hydroxyl radical are still likely to be slow relative to the atmospheric reactions of many organic compounds because of the NHC's low pi-electron density.

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Separations by Reversible Chemical Association*

C.J. King, A.S. Kertes, D. Arenson, J. Tamada, W. Rixey, A. Garcia, L. Poole, and M. Ng

Carboxylic acids, alcohols, glycols and related polar-organic substances are potentially attractive for manufacture from biomass by fermentation. These products must be recovered from highly dilute and complex solutions. Separations based upon reversible chemical association (complexation), using reactive extractants or sorbents, offer better selectivity and lower energy consumption than occur for approaches involving evaporation or distillation of water.

This research involves measurement, modeling and interpretation of phase equilibria and transport for these separations. Further goals are to define rational criteria for selecting complexation reagents, to develop suitable methods for regeneration, and to define the most likely applications. These goals require both chemical and process insight.[1,2]

A related sub-project has explored the use of non-wetting, non-functional macroreticular polymeric adsorbents for selective recovery of these same solutes from dilute aqueous solutions.

The initial phase of the project included literature surveys of the extraction chemistry of carboxylic acids and alcohols.[3,4]

ACCOMPLISHMENTS DURING FY 1987

Extraction of Carboxylic Acids

Equilibria have been measured for extraction of succinic, acetic, lactic and malonic acids by mixed trioctyl and tridecyl amines, with either methyl isobutyl ketone, chloroform or n-heptane as diluent. The results have been rationalized through chemical modeling[5] and show (a) favorable extraction equilibria, (b) overloading of the amine with acid, (c) a molar ratio of water to extracted acid that is different for different carboxylic acids, and (d) substantial effects of temperature and the nature of the diluent.

Three methods for regenerating low-volatility acids from amine extractants have been investigated experimentally – changing temperature to create a more favorable equilibrium for back-extraction into water, changing the composition of the diluent between forward- and back-extraction for the same purpose, and back-extraction into aqueous ammonia, followed by concentration of the aqueous solution and thermal decomposition of the ammonium carboxylate. Studies of regeneration by the latter method have shown that amides are formed irreversibly when ammonium carboxylates are heated. We have now improved this method by replacing ammonia with trimethylamine, which cannot form amides.

Extraction of Alcohols

We earlier found that phenols are effective extractants for alcohols. Equilibria have been measured for extraction of ethanol from aqueous solutions by m-cresol and other phenolic extractants with various diluents, and are being interpreted through chemical modeling.[6] The results so far suggest a 1:1 complex between ethanol and the phenolic extractant. The experiments, modeling and interpretation are complicated by the large number of competing equilibria, and the fact that the various hydrogen bonds formed among alcohols, phenols, water and many of the diluents are of comparable strengths.

The addition of alkyl or halogen substituents to a phenolic extractant has a relatively small effect upon the molar equilibrium distribution coefficient.

Functionalized Polymeric Sorbents

Solid sorbents are potentially non-contaminating. A number of basic polymeric sorbents were tested for recovery of acetic acid from aqueous solution. Properties measured included equilibrium sorption capacity, water uptake, and regenerability either by solvent leaching or by heating and vaporization. The sorbents contained primary, secondary and tertiary amine, pyridyl, amide, N-oxide, and imidazole functional groups.

Equilibrium sorption capacities have been successfully interpreted through a chemical-exchange model, relating the capacity to the density of accessible functional groups and an affinity constant related to the basic strength, as represented by the Gutmann Donor Number. Water is taken up by pore filling and swelling. Swelling has been related to osmotic pressure.

Exploratory studies have been made of regeneration of acetic acid from amine, pyridyl and imidazole resins. Pyridyl sorbents can be regenerated by common solvents (e.g., methanol) at ambient tem-

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Energy Systems Research, Energy Conversion and Utilization Technologies (ECUT) Division of the U. S. Department of Energy under Contract No. DE-AC03-76SF00098.

perature, but the other basic groups are much less amenable to regeneration by solvent leaching.

Dowex WGR, a high-capacity amine sorbent, can be regenerated by aqueous ammonia solution, which can be followed by thermal decomposition of the ammonium carboxylate to enable recovery of the carboxylic acid and recycle of ammonia. Again, it may be desirable to use a low-molecular-weight tertiary amine rather than ammonia, so as to avoid amide formation.

Thermal degradation hampers regeneration of polymeric sorbents by heat and vaporization. However, Dowex MWA-1, a high-capacity tertiary amine sorbent, can be regenerated by heating to 100°C for several hours. Celanese Aurorez, a polybenzimidazole, is stable to very high temperatures but undergoes a surface-sealing phenomenon if heated in the presence of imbibed water. These results suggest several avenues for improved regeneration.

Non-Wetting Adsorbents

Because of low water uptake, non-wetting macroreticular styrene-divinylbenzene adsorbents are potentially attractive for recovery of polar organics from dilute aqueous solution. Since the rate-limiting step is Knudsen diffusion within air-filled pores, these adsorbents can also fractionate among solutes with different volatilities.[7]

Fixed-bed studies with non-wet adsorbents showed that it is important to purge interstitial air with water before introducing the feed to be fractionated. The degree of separation among components was interpreted quantitatively by allowance for axial dispersion and rates of Knudsen diffusion within the pores.[8]

PLANNED ACTIVITIES FOR FY 1988

Regeneration of Extractants and Adsorbents

Improved regeneration is the greatest need for economical recovery of carboxylic acids by complexing extractants or sorbents. The thermodynamics of extraction of carboxylic acids by tertiary amines will be examined to seek ways of obtaining large effects of temperature and/or diluent change upon extraction equilibria, thereby facilitating regeneration by back-extraction following changes in temperature and/or diluent.

Phase equilibria will be determined for regeneration of amine extractants and sorbents by back-extraction with aqueous trimethylamine, and thermal decomposition tendencies of the resulting trimethylammonium carboxylates will be measured. Two additional regeneration methods to be explored are precipitation of low-solubility carboxylic acids (e.g., fumaric) and displacement of extracted or sorbed carboxylic acid by a stronger acid, which is more readily regenerated. Improved thermal regeneration of poly(benzimidazoles) will be sought through methods which avoid or reduce surface sealing.

Extractants and Sorbents

Systematic development of improved sorbents will be pursued by complementing chemical insight with improved understanding of the effects of the morphology of the solid on capacity, water uptake and regenerability.

Extraction equilibrium data will be obtained for additional carboxylic acids, so as to enable generalizations about affinity constants and tendencies for overloading of amine extractants, co-extraction of water, and regeneration by various means. Spectroscopic measurements will be made where appropriate and useful for confirming association stoichiometry. Extraction equilibria for recovery of glycols with phenolic extractants will be measured and interpreted, and stronger extractants for alcohols and glycols will be sought. Sorbents or polymeric extractants with pendant phenol groups (e.g., polyvinylphenol) will be investigated for recovery of alcohols and glycols.

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Differential Photothermal Deflection Spectroscopy*

R.E. Russo, J.D. Spear, and R.J. Silva†

Photothermal deflection spectroscopy (PDS) has been recognized for its ability to measure ultrasensitive radiative absorption in transparent media. Unlike conventional beam-transmittance spectrophotometry, PDS directly measures the absorbed radiation by monitoring temperature gradients produced within the medium. However, for liquid-phase analysis, absorption by the solvent (background) limits the sensitivity of analysis. We developed a dual-beam, differential PDS system using a split probe-beam arrangement with a single position sensor and detection electronics to correct for background absorption.

ACCOMPLISHMENTS DURING FY 1987

The optical arrangement of this PDS system is shown in Fig. 1. An argon-ion pumped dye-laser, modulated at 80 Hz, provided the excitation radiation. A linearly polarized helium-neon laser served as the probe-beam source. The excitation and probe lasers strike opposite sides of a dielectric beam splitter at nearly equal angles of incidence. The beam splitter produced two sets of excitation and probe beams which overlap in a sample cuvette (S) and a reference cuvette (R). Lenses (L_1 and L_2) are placed before the beam splitter and focus the excitation and probe beams in the centers of the cuvettes. Within each cuvette, both the excitation and probe beams are horizontal, intersecting each other at an angle of ~0.5°. The axis of the probe beam is aligned slightly above that of the excitation beam. The position detector is a single-axis, solid-state, photodetector with an attached interference spike filter that passes only the light from the HeNe probe beam. The position detector signal is conditioned and fed into a lock-in-amplifier.

The conventional PDS approach is to monitor the deflection of both beams with two separate position detectors and additional related electronics. However, this approach is limited because of electronically subtracting uncorrelated signals. Our PDS system avoided this problem by folding the reference probe beam back into the path of the sample probe beam so that only a single position detector was needed (cf. Fig. 1). Two mirrors (M_1 and M_2) and a prism (P) allowed the two probe beams to overlap on the detector. The placement of an additional lens

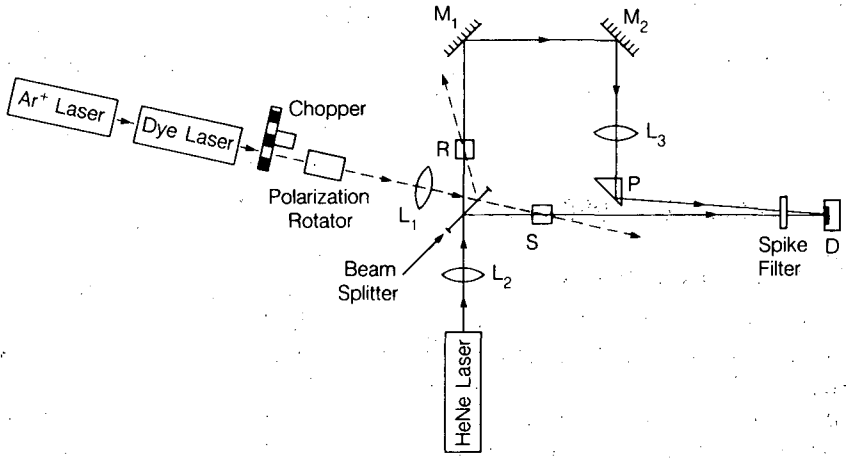

Figure 1. Optical arrangement of the dual-beam, differential photothermal deflection spectroscopy (PDS) system. (XBL 8711-9102)

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† Nuclear Chemistry Division, Lawrence Livermore National Laboratory.

(L_3) in the reference beam path was necessary to make its deflection subtractive, rather than additive, to that of the sample probe beam.

If the relative intensities of the reference and sample probe beams at the detector are equal, then the position sensor measures their average deflection. Because the reflectance of the beam splitter depends on the polarization of incident light, these relative intensities were balanced by rotating the cylindrical probe laser head about its longitudinal axis until the beam's polarization was near 45° from vertical. Similarly, an adjustable polarization rotator was placed before the beam splitter to balance the relative intensities of the excitation beams in the reference and sample cuvettes, so that comparable deflection amplitudes would result when the two cuvettes contained similar solutions.

Background correction and sensitivity were demonstrated by using a dilute solution (10^{-5} M) of Nd^{3+} in 10^{-2} M HCl. Neodymium has a narrow absorption line at 575 nm with a molar absorptivity of only 6.9 L $mole^{-1}cm^{-1}$. The reference cell contained only the solvent. The spectra in Fig. 2a were obtained by alternately removing the reference and the sample solutions. The absorption of 10^{-5} M Nd^{3+} in HCl (I) provided a positive deflection signal, while the absorption of the reference HCl (II) provided a negative deflection signal. The background absorption of the solvent obscured the absorption spectrum of the neodymium at this concentration. However, when the system was operated with both solutions in place, the correct absorption spectrum for 10^{-5} M Nd^{3+} was measured (Fig. 2b). Thus, real-time, differential background correction provided an increase in PDS sensitivity.

PLANNED ACTIVITIES FOR FY 1988

A differential dual-beam thermal lensing spectroscopy (TLS) system will be developed and compared to the PDS system. In addition, the possibility of performing TLS and PDS at the end of optical-fibers will be explored.

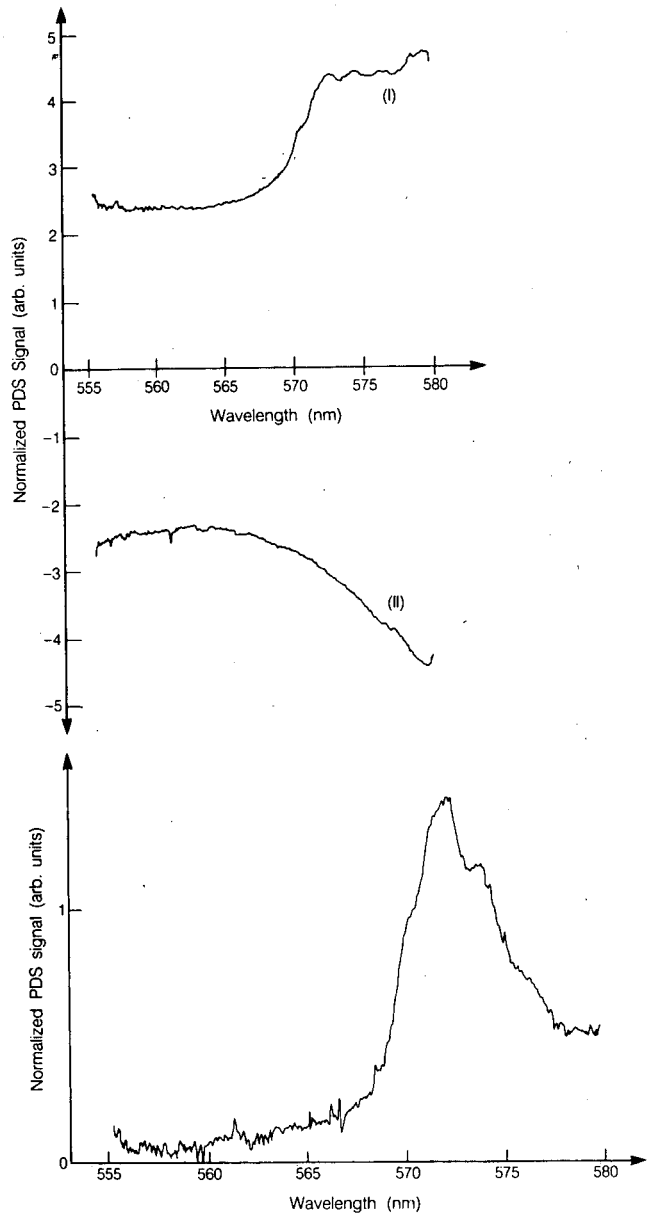

Figure 2. PDS signal for a) 10^{-5} M Nd^{3+} (I) and 10^{-2} M HCl (II) without background correction, and b) with background correction. (XBL 8711-9100A)

ENVIRONMENTAL RESEARCH PROGRAM

INTRODUCTION

The principal objective of the Environmental Research Program is to understand the formation, transformation, transport, and effects of energy-related pollutants on the environment, and how these are influenced by energy generation and emission control technology. Because a comprehensive understanding of these processes is crucially dependent on experimental data, a substantial effort in the Program is devoted to development and application of state-of-the-art measurement and analytical methods. This multidisciplinary research program includes fundamental and applied research in physics, chemistry, engineering, and biology, as well as research on the development of advanced methods of measurement and analysis. The Program's Annual Report contains summaries of research performed during FY 1987 in the areas of atmospheric aerosols, flue gas chemistry, combustion, membrane bioenergetics, and analytical chemistry.

The main research interests of the Atmospheric Aerosol Research Group concern the chemical and physical processes that occur in haze, clouds, and fogs. For their studies, the group is developing novel analytical and research methods for characterizing aerosol species. Aerosol research is performed in the laboratory and in the field. Studies of smoke emissions from fires and their possible effects on climatic change, especially as related to nuclear winter, are an example of the collaboration between the Atmospheric Aerosol Research and Combustion Research Groups.

The Flue Gas Chemistry Research Group is engaged in research whose aim is to help develop new processes for simultaneous SO_2 and NO_x removal. Current research is directed toward understanding the kinetics and mechanisms of homogeneous and heterogeneous catalysis of the interactions of sulfur dioxide and nitrogen oxides, both among themselves and with other compounds. When this fundamental chemistry is understood, it will be applied to the development of an efficient, cost-effective scrubber for simultaneous desulfurization and denitrification of flue gases.

The Combustion Research Group studies complex combustion processes by acquiring a fundamental understanding of the physical and chemical processes that determine the combustion efficiency, formation, and emissions of species from these processes. Controlled combustion studies have a goal of developing means whereby the zone of chemical activity would be spread out, so that its distribution in space and time could be controlled. The characterization and understanding of turbulence and its relationship to the combustion process are studied in simplified laboratory-scale burners using advanced laser diagnostic techniques. Combustion chemistry studies center on the theoretical understanding of thermal and state-to-state reactions with the purpose of characterizing elementary reactions and developing predictive capabilities.

The Membrane Bioenergetics Group studies the effects ofof strongly chemically reactive compounds generated within cells. Specific research efforts in FY 1987 were in photochemical conversion of solar energy by microbial systems. They are currently investigating biological oxidation and bioenergetics of cyanobacteria, bacteriorhodopsin, and bacterial succinate dehydrogenase. Another area of the Group's interest is in development and application of new assays of oxidation damage by using free radical measurements that arise during normal metabolism and under pathological conditions.

One of the main emphases in Analytical Chemistry has continued to be in the area of asteroid impacts and mass extinctions. The nature of the sedimentation of the rocks, the worldwide extent of the extinction horizons, and the extent to which the extinctions are related to impacts are also studied. Another area of emphasis is the application of synchrotron radiation to the analysis of minute amounts of trace elements in a variety of environmental and other samples.

The short reports that follow describe the program activities in FY 1987. For many of these reports, more detailed papers have been or will be published in appropriate scientific journals.

Incorporation of Soot Particles into Droplets*

W.H. Benner, A.D.A. Hansen, and T. Novakov

The incorporation of particles into fog or cloud droplets is influenced by factors such as particle size, composition, and the supersaturation of water vapor. For soot particles, their size and composition are affected by combustion conditions and fuel composition. Because fossil fuels contain differing amounts of sulfur, some of which is converted into particulate sulfate during combustion, its concentration in the fuel critically affects the nucleation properties of soot particles. Using a previously described chamber,[1] we have continued to study the influence of fuel sulfur on soot particle composition and on the nucleation of soot particles. By introducing SO_2 and NH_3 into the soot particle-droplet reaction system, we have also been able to study the influence of heterogeneous sulfate formation.

ACCOMPLISHMENTS DURING FY 1987

A two-channel aethalometer[2] has been used to determine the total and interstitial concentrations of black carbon in the fog chamber as a function of fuel sulfur content. In Fig. 1, the line drawn through the solid circles indicates the fraction of black carbon incorporated into droplets as a function of the total black carbon concentration for soot particles produced by the combustion of nearly sulfur-free propane. As the black carbon concentration increased, the fraction incorporated into droplets decreased because a fixed amount of water vapor that is available for droplet formation has to be distributed among the active nuclei. The line drawn through the boxes in Fig. 1 shows the incorporation of black carbon produced from propane fuel that contained 2.5% (wt/wt) sulfur. The fraction of black carbon incorporated into droplets also decreased as the black carbon concentration increased, but the effect of fuel

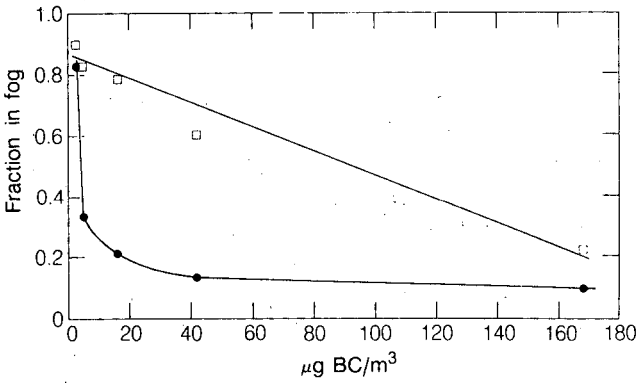

Figure 1. The effect of fuel sulfur on the incorporation of black carbon particles. The solid circles indicate the mass fraction incorporated into droplets for nearly sulfur-free propane combustion particles. For similar nucleation conditions, the boxes indicate that increased incorporation occurs for soot particles produced by the combustion of propane containing 2.5% (wt/wt) sulfur. (XBL 882-8362)

sulfur is obvious. The cause for the increased incorporation is an increase in the particulate sulfate/black carbon ratio that occurred with enrichment in fuel sulfur. The results led us to hypothesize that soot particles from sulfur-rich fuels have shorter atmospheric lifetimes than soot particles from sulfur-poor fuels.

Studies were conducted in which the concentration of particulate sulfate in the chamber was measured as a function of $[NH_3]$, $[SO_2]$, and black carbon concentration. The presence of NH_3 in this heterogeneous reaction system significantly increased the formation of particulate sulfate—a result that was not observed in the absence of droplets and/or soot particles. In the presence of droplets, the formation of particulate sulfate depended strongly on the black carbon concentration.

PLANNED ACTIVITIES FOR FY 1988

We plan to continue these studies so that the heterogeneous reactions of NH_3, SO_2, soot, and droplets in the atmosphere can be described kinetically.

*This work was supported by the Director, Office of Energy Research, Office of Health and Environmental Research, Physical and Technological Research Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, and by the National Science Foundation under Contract ATM 8713712.

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1. Benner, W.H., Hansen, A.D.A., and Novakov, T. (1987), *FY 1986 Annual Report of the Environmental Research Program*, Lawrence Berkeley Laboratory report LBL-22154, p. 4-7.

2. Hansen, A.D.A., Rosen, H., and Novakov, T. (1984), "The Aethalometer—An Instrument for the Real-Time Measurement of Optical Absorption by Aerosol Particles", *Sci. Total Environ. 36*, p. 191.

The Incorporation of Ambient Carbonaceous Aerosols in Advection Fog*

A.D.A. Hansen and T. Novakov

Aerosol black carbon is a ubiquitous pollutant species produced by incomplete combustion. In addition to impacts on visibility and the solar radiation balance, caused by its large optical absorption, it may also participate in heterogeneous-phase reactions of importance in atmospheric chemistry. The oxidation of SO_2 to sulfate in a water film on a carbon surface has been demonstrated in the laboratory. However, it was generally believed that ambient carbonaceous aerosols are hydrophobic, and therefore the contribution of this mechanism to aerosol acidification was of unknown significance. In this article we present the results of a field study showing that up to 80% of the ambient black carbon aerosol can be found incorporated into fog droplets.

ACCOMPLISHMENTS DURING FY 1987

To study the incorporation of aerosol black carbon into fogs, we used a two-channel aethalometer to measure this aerosol component in real time. One channel sampled the total aerosol through an open probe, heated to evaporate any fog water. This channel therefore measured both the interstitial aerosol and any black carbon that had been occluded by fog droplets. The other channel was preceded by several layers of nylon mesh, which served to impact any particles of aerodynamic diameter greater than 1 μm, and therefore to remove any droplets. This channel therefore measured only the interstitial aerosol. The presence of fog was detected semi-quantitatively by an infrared transmissometer.

This equipment was set up at U.C. Davis during January and February, 1987, to study radiation fogs common in winter in the central California valley. Unfortunately, an unsuitable location and abnormal winter meteorology resulted in very little fog being sampled. In August and September, 1987, the equipment was set up at LBL to study marine advection fogs common in the Bay Area in summertime. Figure 1 shows the incorporation of aerosol black carbon as a function of time during a fog impact; Fig. 2 shows the incorporation fraction vs. total black carbon concentration for 20-min data averages during both foggy and clear periods. It is clear that at low aerosol concentrations, a majority of the black carbon is indeed occluded by fog droplets. The transit times of these particles from the urban source regions to LBL were short ($\leq$ 1 hr), implying that this hygroscopicity is an attribute of the primary aerosol.

PLANNED ACTIVITIES FOR FY 1988

In collaboration with U.C. Davis, the equipment will be set up at a more suitable location in flat open terrain to study wintertime radiation fog in the central California valley.

*This work was supported by the National Oceanic and Atmospheric Administration under contract 40 RANR 520248, Coordinating Research Council, and the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

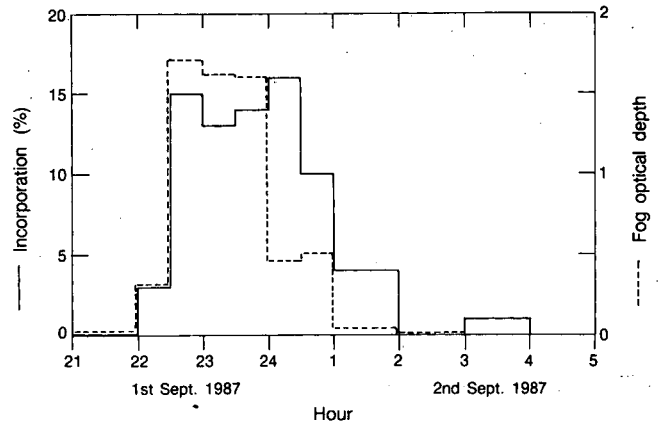

Figure 1. Fraction of ambient black carbon aerosol incorporated into fog droplets during marine advection fog episodes, plotted vs. total black carbon concentration. Each point represents a 20-min average of the continuous data for sampling times during a 7-day interval. Data for both foggy and clear periods are shown. (XBL 881-9625)

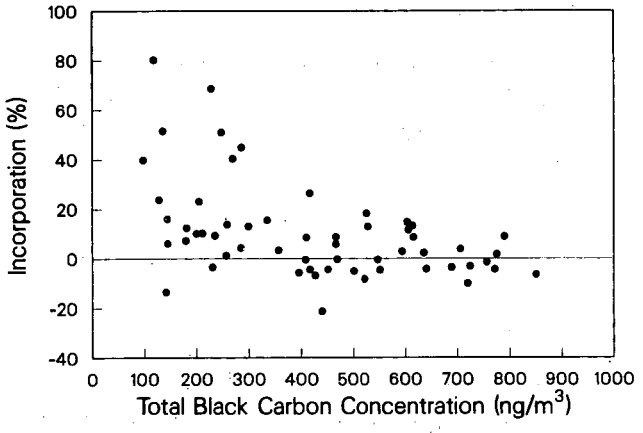

Figure 2. Fraction of ambient black carbon aerosol of size smaller than 0.3 μm, relative to total concentration. Data averaged by hour (local time) for 27 days in June and July at Claremont College, California (1987 summer SCAQS program). (XBL 879-11386)

Development of Real-Time Measurement Capability for Particulate Ammonium, Sulfate, and Nitrate*

L.A. Gundel and T. Novakov

The inorganic ions ammonium, sulfate, and nitrate are among the principal components of atmospheric particles. To begin to develop real-time measurement capability for these species, ambient particles were collected on Teflon filters while their absorbance was continuously measured, using Fourier transform infrared spectroscopy. Measurements of concentrations of NH_4^+, $SO_4^=$, and NO_3^- are currently performed routinely by ion chromatographic analyses of water extracts of filter samples of particles. Besides involving time-consuming sample preparation steps, this destructive technique may not actually reflect the original composition of the particles because of subsequent chemical changes on the filters. Another drawback of extraction-based analytical methods is the limit of detection. For $SO_4^=$, ion chromatography requires sampling times of at least 4 hr to obtain loadings > 1 $\mu g/cm^2$ on the filter.

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ACCOMPLISHMENTS DURING FY 1987

Figure 1 shows infrared absorbance due to NH_4^+, $SO_4^=$, and water for particles collected from ambient room air after 20 min of sampling. Using a sampling

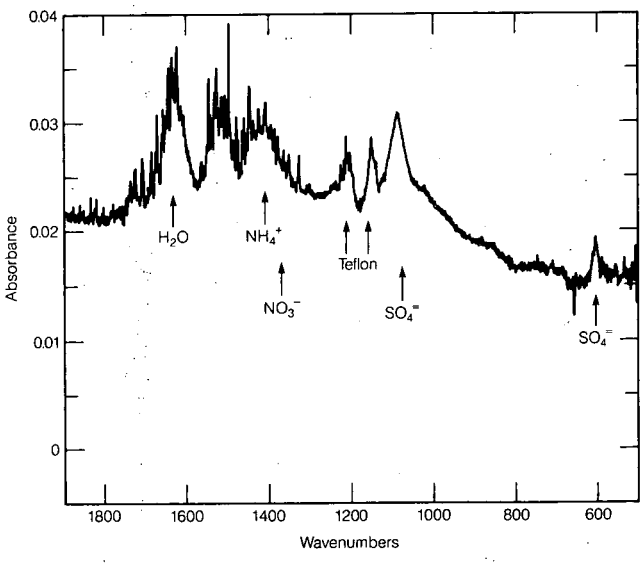

Figure 1. Infrared absorbance of ambient indoor particles, collected on a Teflon filter after 20 min of sampling. (XBL 882-11001)

rate of 20 liters/min and a collection area of 1 cm^2, the nondestructive FTIR technique detected $SO_4^=$ at $\leq$ 0.05 $\mu g/cm^2$ with a sampling time of 10 min or less. This is at least 20 times more sensitive for $SO_4^=$ than ion chromatography.

PLANNED ACTIVITIES FOR FY 1988

Measurements of the sensitivity of the method for NH_4^+ and NO_3^- will be made. The technique will be used to monitor particulate NH_4^+, $SO_4^=$, and NO_3^- indoors and outdoors.

The Interaction of NO_2 with Carbon Particles*

L.A. Gundel and T. Novakov

Both nitrous and nitric acids are found in polluted air. Nitric acid is an important component of acid deposition; nitrous acid may be a health hazard and pathways for its production in the atmosphere here have not yet been identified. This work explores the potential for carbon particles to play a role in heterogeneous production of NO_2^- and NO_3^- in the atmosphere and in indoor environments.

ACCOMPLISHMENTS DURING FY 1987

The interaction of NO_2 in air (0.5-35 ppm) with 20-mg carbon particles led to three products: NO, detected in the gas phase, and NO_2^- and NO_3^-, removed from the particles by water extraction. Figure 1 shows that the relative amounts of these products depended on the NO_2 concentration and the presence of water. At 4 ppm or below, in dry or humid air, the product distribution, in relative molar amounts, was $NO_3^- = 2NO_2^- = 2NO$. At 20 ppm and above, the relative amounts of products depended on the presence of water vapor: in dry air $NO = 3NO_3^- = 6NO_2^-$; in humid air $NO = NO_2^- = 2NO_3^-$. For carbon slurries in water, $[NO_2^-] = 6[NO_2^-]$ at an input concentration of NO_2 of 4 ppm. In comparison to carbon, alumina particles and glass beads removed NO_2 ineffectively. At 4 ppm carbon removed 97%, while alumina and glass removed 8 and 0% of the input NO_2 respectively.

These results indicate that NO_2 oxidized the carbon particles while it was reduced to NO. NO_2 adsorbed at oxidized sites on the particles formed a

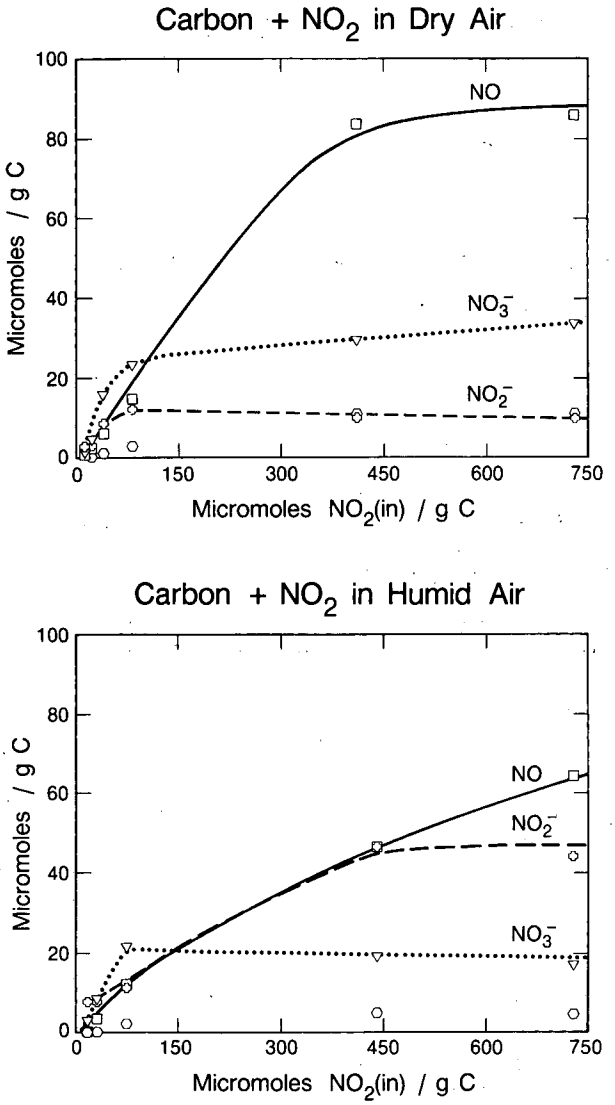

Figure 1. Amounts of nitrogenous species resulting from the interaction of NO_2. Upper: NO_2 in dry air; lower: NO_2 in humid air (50% relative humidity). Hexagons represent NO_2 measured downstream of the reaction vessel. (XBL 881-8806A)

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surface species that was analyzed as nitrate. When NO_2 adsorbed at other (nonoxidized) sites, equal amounts of NO_2^- and NO_3^- formed, as expected from reactive dissolution behavior of NO_2. At high enough concentrations of NO_2 (20 ppm and above), the interaction of NO with the surface nitrate produced NO_2^-. In slurries, NO, generated from interaction of NO_2 with carbon, reacted with surface nitrate or nitric acid in solution to form the relatively large quantities of nitrite observed here. This work suggests that NO_x reactions with carbon in droplets or on wet surfaces could be important sources for the production of nitrous acid in the environment; on dry particles both nitrous and nitric acids could be formed by this pathway.

PLANNED ACTIVITIES FOR FY 1988

We plan to continue this work with carbon, combustion soot, urban particulate matter, and slurries of typical fog water composition. The rates of production of NO, NO_2^-, and NO_3^- will also be measured.

Smoke Emissions from Medium-Scale Oil Pool Fires*

R.L. Dod, R.B. Williamson, N.J. Brown, and T. Novakov

Evaluation of the potential significance of a "nuclear winter" produced by smoke from post-nuclear exchange fires depends largely upon the quantity of smoke generated, its distribution in the atmosphere, and its optical characteristics.[1] Existing information regarding these factors is insufficient to reliably estimate the effects of such fires.[2] It is considered that smoke contributions from burning of petroleum stocks may be a major contributor to the climatic effects due to fuel concentration and smoke emissions factors. We have extended our previous measurements of emission factors and size distributions for smoke from burning urban building materials[3] to include emissions from fuel oil pool fires under both free-burning and ventilation-restricted conditions.

ACCOMPLISHMENTS DURING FY 1987

The series of experiments conducted this year were primarily with fuel oil pool fires. Both fire scale and ventilation conditions were varied to produce a data set from which extrapolation to large-scale fires could be reasonably done. The oil was burned in pools 56 cm in diameter, either individually or in two similar pools side by side. Single 56-cm pools were also burned in the "burn room," a fire-resistant, enclosed room at the University of California's Fire Research Laboratory.

Average measured emission factors (smoke particle mass as a fraction of fuel consumed) are shown in Fig. 1, together with those for building materials determined previously. The smoke generated from burning single pans of oil exceeded 10% of the consumed fuel mass, a fraction that is in general agreement with that from burning asphalt roofing. When the fire intensity was increased by burning two pools

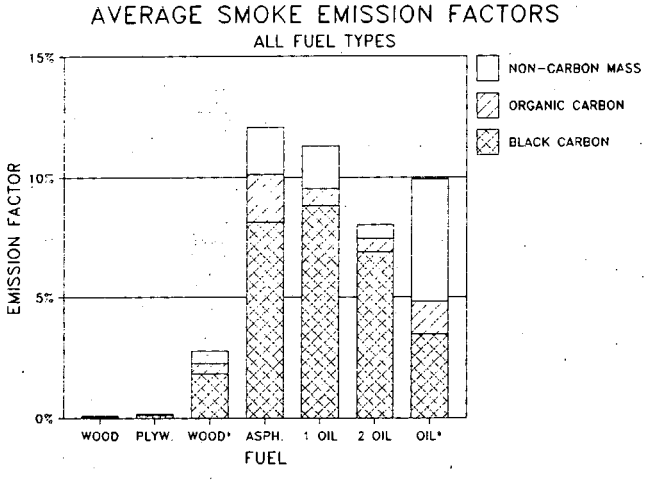

Figure 1. Measured average emission factors for all fuel types. WOOD refers to solid wood, PLYW. to plywood, and ASPH. to asphalt roofing shingles. WOOD* and OIL* refer to fuels burned under restricted ventilation conditions. (XBL 882-546)

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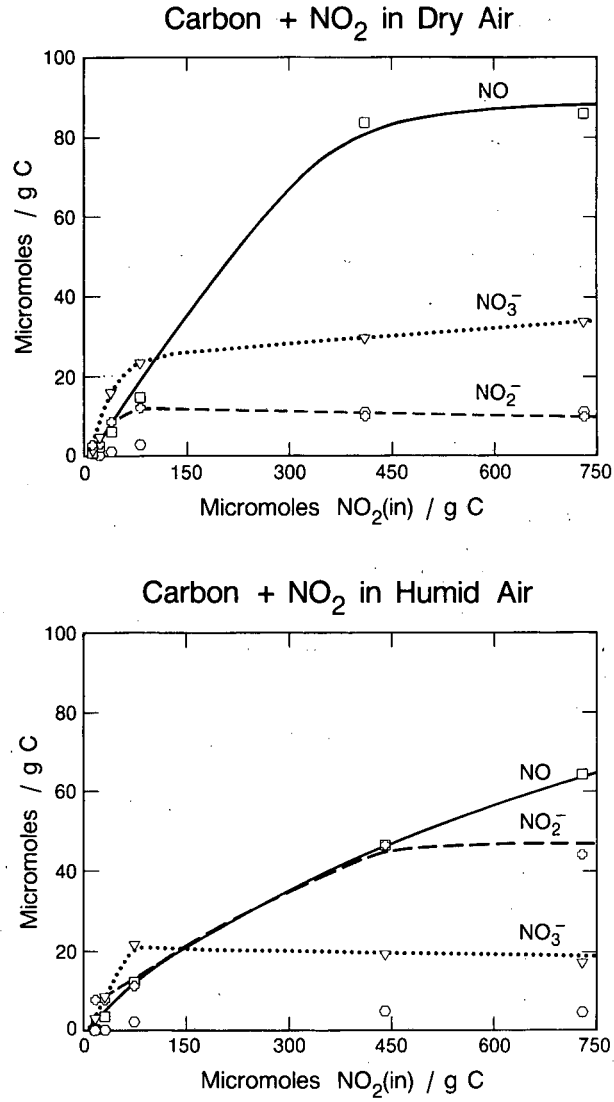

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R.L. Dod, R.B. Williamson, N.J. Brown, and T. Novakov

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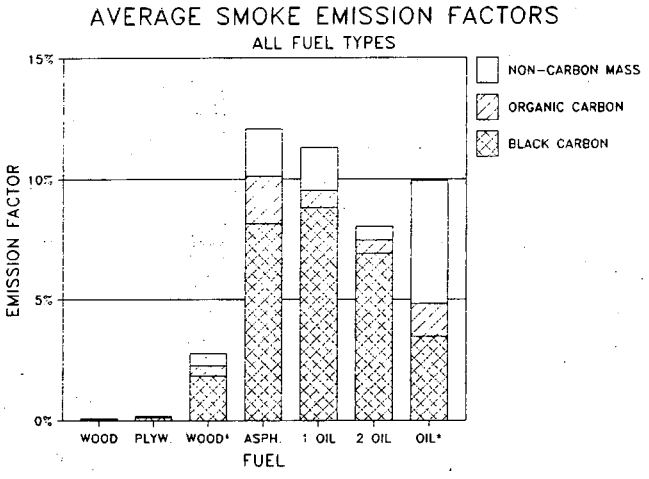

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of oil side by side, smoke emissions dropped by a reproducible amount. Whether this change will hold with further increase in scale or change of configuration is not known. Soot carbon emissions from oil burned under ventilation restricted conditions were approximately 50% less than was observed for similar scale fires in the open. (The large non-carbon smoke mass in these experiments is probably from the lining of the burn room or the antechamber, which was also involved in fire from pyrolyzates during flashover.) We do not know why there is a decrease in emission factor when oil is burned under limited ventilation conditions, while wood burned in a similar fashion shows a dramatic increase in emissions.

Particle size distributions for the fires in the open showed the largest fraction to be less than 0.3 μm aerodynamic diameter, although a secondary peak was apparent in the distribution functions at 1-2 μm. As with underventilated wood fires, the particle mass peak shifted into the 1-2 μm range, with few fine particles present. This shift in particle size is potentially important to the prediction of climatic effects, since Penner[4] has calculated that particles >1 μm diameter are much more susceptible to incorporation into water droplets and thus potentially to rainout than are particles in the 0.1 to 0.3 μm size range.

PLANNED ACTIVITIES FOR FY 1988

We intend to continue this work with further exploration of the effects of scaling, fuel geometry, and composition to the extent that our facility will allow.

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4. Penner, J.E., "Predicting the Consequences of Nuclear War," *3rd International Conference on Carbonaceous Particles in the Atmosphere*, October 3-8, 1987, Berkeley, California.

Single Submicron-Sized Particle Analysis*

W.H. Benner and R. Otto

Currently available information on the composition of individual submicron particles is extremely limited. This information is useful because currently available techniques provide composition data that can only be reported as an average of all particles, even though individual particles in a sample can have greatly differing compositions. Particle analysis in real time will provide additional benefits, one of which is the preclusion of particle contamination (artifact formation) during sample collection time.

*This work was supported by the Director, Office of Energy Research, Office of Health and Environmental Research, Physical and Technological Research Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

ACCOMPLISHMENTS DURING FY 1987

We have started a new project in which a method to analyze individual particles in real time for elemental composition is being developed. Particles in the diameter range of 0.01 to 10 μm will be electrically charged and accelerated to velocities such that their impact with a target will produce a plasma. The plasma will be analyzed by mass spectrometry for elements.

Charged test particles of activated carbon, polystyrene spheres, sodium chloride, and fluorescent dyes were generated and drawn into a sonic velocity accelerator (Fig. 1). This differentially pumped capillary-skimmer system was built and tested as a way to produce a well-defined beam of particles in vacuum and is to be used eventually to inject particles into a 100-kv electrostatic accelerator. Performance tests showed that as the particle beam exited the skimmer, it diverged only 0.2°. The velocity of the particles in the beam was measured by use of

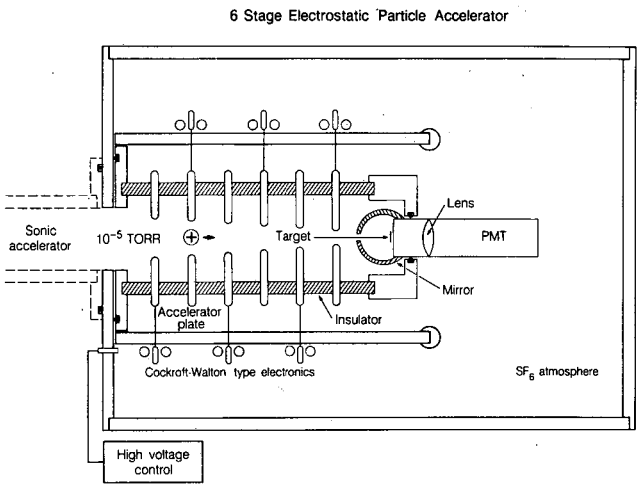

Figure 1. Schematic of a sonic velocity accelerator in which a capillary-skimmer system is used to produce a beam of test particles in vacuum. (XBL 881-8337)

two rotating disks. A hole in the first disk chopped the beam; and the second disk, spaced 8.5 cm from the first, was used to collect particles by impaction. Measurement of the disks' rotational speed and the angular displacement of the beam spot from a center line position on the second disk showed particle velocity to be ~ 300 m/sec or ~ 95% of sonic velocity. This particle velocity indicated that the differentially pumped capillary skimmer was working without fluid flow disturbances and will provide a way to inject electrically charged particles into an electrostatic accelerator that is currently under construction.

PLANNED ACTIVITIES FOR FY 1988

We plan to continue to develop this analytical technique. The sonic accelerator will be coupled to a 100-kv electrostatic accelerator, and we will attempt to detect high velocity particle impact events.

Reaction of Nitric Oxide with Fe(II) Complexes of SH-Containing Amino Acids*

D.K. Liu, D. Littlejohn and S.G. Chang

Conventional ferrous chelates employed in wet flue gas scrubbing systems to promote NO removal include Fe^{2+}(EDTA) and Fe^{2+}(NTA). We recently reported a process using ferrous cysteine as additive which possesses several advantages over the conventional Fe^{2+}(EDTA)-type chelates.[1] We have since extended our effort to include ferrous chelates of other SH-containing amino acids and peptides.

ACCOMPLISHMENTS DURING FY 1987

We have discovered that ferrous chelates of N-acetylcysteine (AcCySH), penicillamine (Pen), N-acetylpenicillamine (AcPen), glutathione (GSH), and cysteinylglycine (cys-gly) are more effective in NO removal compared to that of cysteine (CySH).[2] The experiments were carried out at 55°C and between pH 4.3 and 12.0 by bubbling a gaseous mixture of NO(P_{NO} = 500 ppm), O_2 (4%) and N_2 (balance) into an absorber containing a buffered solution of ferrous salt (0.01 M) and amino acid/peptide (0.04 M). The results are shown in Figure 1. While the NO absorption capacity of $Fe^{2+}(CyS)_2$ is fairly insensitive to pH, $Fe^{2+}(Pen)_2$, $Fe^{2+}(AcCyS)_2$, and $Fe^{2+}(AcPen)_2$ are most efficient in neutral solutions (pH $\sim$ 7) and become ineffective in acidic (pH $<$ 6) or strongly alkaline (pH $>$ 11) medium. The ferrous peptide complexes behave somewhat differently from the amino acid complexes. The maximum NO removal capacity for Fe^{2+}(GS) was found at pH 5.4, with nNO/nFe^{2+} = 0.54. The $Fe^{2+}(cys\text{-}gly)_2$ system absorbed NO under all conditions studied. The nNO/nFe^{2+} ratio was 0.28 between pH 4.3 and 5.5, rose to 0.87 at pH 7.3, and then dropped off rapidly as the pH increased, falling to 0.05 at pH 9.2.

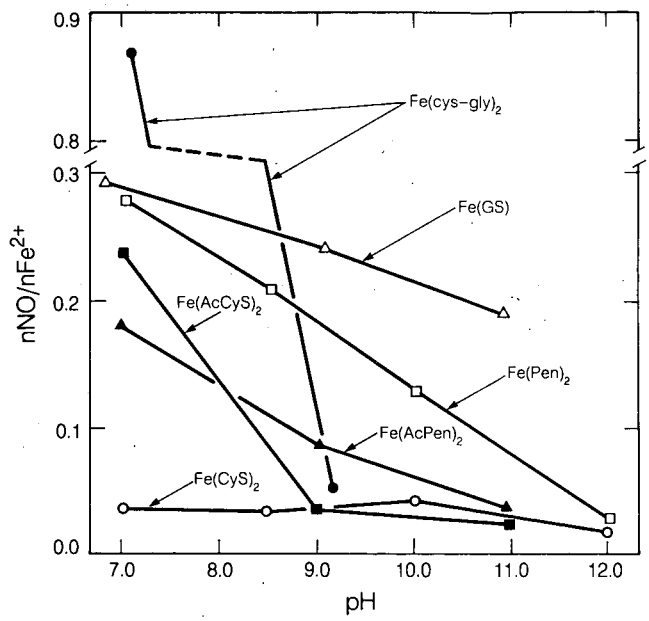

Figure 1. The NO absorption capacity of ferrous thioamino acid/-peptide complexes as a function of pH. (XBL 8711-9339)

The fate of the absorbed NO was determined by vacuum line experiments at pH 7.0 in the absence of O_2. In the case of $Fe^{2+}(CyS)_2$, 46% of the absorbed NO was reduced to a $\sim$ 1:1 mixture of N_2 and N_2O, with the remaining of the absorbed NO in a $Fe(CySSCy)(NO)_2$ precipitate. For $Fe^{2+}(Pen)_2$, all of the absorbed NO was reduced to N_2 ($\sim$ 91%) and N_2O ($\sim$ 9%) in the gas phase. In the Fe^{2+}(GS) system, all of the absorbed NO was converted to a mixture of NO_2^- ($>$ 85%) and NO_3^- (5-15%) in solution. The different NO-derived products imply different mechanisms are involved in the ferrous amino acid and peptide systems. Finally, we have found that the disulfide forms of CySH, AcCySH and GSH obtained after NO absorption can be reduced back to the starting thiols using a simple and potentially cost-effective method involving $H_2S/SO_2/OH^-$. For the regeneration of thiols from the disulfides of Pen, AcPen and cys-gly, electrochemical reduction appears to be the only viable method at present.

PLANNED ACTIVITIES FOR FY 1988

The study of these systems has been completed and no further work is planned.

*This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal Utilization Systems, U.S. Department of Energy under Contract No. DE-AC03-76SF00098 through the Pittsburgh Energy Technology Center, Pittsburgh, PA.

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Removal of Nitric Oxide from Flue Gas Using Water-Soluble Iron (II) Dithiocarbamates*

D.K. Liu and S.G. Chang

The reaction of metal dithiocarbamates with NO was first reported over fifty years ago. However, the metal dithiocarbamates and their nitrosyl complexes prepared thus far are predominantly those containing dialkyl substituents. These metal chelates are only soluble in organic solvents and therefore are not applicable to wet flue gas scrubbing systems in which water is the medium. Recently, it came to our attention that dithiocarbamates containing negatively charged carboxylate substitutents can be prepared by the reaction of glycine (Gly) and iminodiacetic acid (IDA) with carbon disulfide in sodium hydroxide solution. The iron (II) chelates of such dithiocarbamates should be water-soluble and therefore we decided to prepare these chelates and to study their reactions with NO.

ACCOMPLISHMENTS DURING FY 1987

We have prepared sodium N-carboxymethyl-dithiocarbamate via the reaction of Gly and CS_2 in 2.0 M sodium hydroxide solution as shown in equation 1.

$$HO_2CCH_2NH_2 + CS_2 + 2NaOH \rightarrow Na^+ {}^-O_2CCH_2NHCS_2^- Na^+ + 2H_2O \quad (1)$$

Similarly, the reaction of IDA with CS_2 yields bis (N-carboxylmethyl) dithiocarbamate according to equation 2.

$$(HO_2CCH_2)_2NH + CS_2 + 3NaOH \rightarrow (Na^+ {}^-O_2CCH_2)_2NCS_2^- Na^+ + 3H_2O \quad (2)$$

The presence of these dithiocarbamates derived from Gly and IDA (abbr. Gly-dtc and IDA-dtc, respectively) in the reaction mixture was confirmed by the precipitation of these intermediates as S-benzylthiuronate derivatives, and by uv-visible and laser Raman spectroscopies. Using the same method, dithiocarbamates derived from diethanolamine (DEA) and urea (abbr. DEA-dtc and urea-dtc, respectively) have also been prepared.

The removal of NO from a simulated flue gas mixture containing 500 ppm NO and 4% O_2 can be effected by aqueous solutions containing various iron

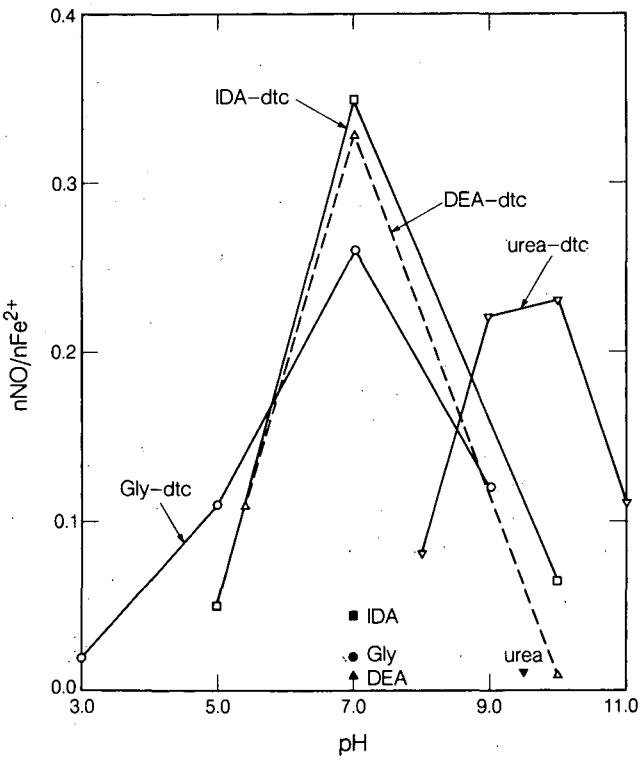

Figure 1. The NO absorption capacity of iron (II) dithiocarbamates as a function of pH. (XBL 8712-9111)

*This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal Utilization Systems, U.S. Department of Energy under Contract No. DE-AC03-76SF00098 through the Pittsburgh Energy Technology Center, Pittsburgh, PA.

(II) dithiocarbamates as shown in Figure 1. Most of the iron (II) dithiocarbamates in this study work best under neutral conditions, with the exception of Fe^{2+}(urea-dtc)$_2$, which is most effective between pH 9.0 and 10.0. Product analyses-showed that most of NO absorbed by Fe^{2+}(Gly-dtc)$_2$ and Fe^{2+}(IDA-dtc)$_2$ solutions ended up as gas phase products N_2 and N_2O in ratios of ~ 4:1 and ~ 10:1, respectively.

PLANNED ACTIVITIES FOR FY 1988

Future efforts will be directed towards the isolation of pure alkali metal salts of the above dithiocarbamates for use in the absorbent solutions, complete characterization of the iron dithiocarbamates, and the extension of the present concept to xanthates and thioxanthates.

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Development of Reagents for Use in Spray-Drying Systems to Control SO_2 and NO_x Emissions*

D. Littlejohn and S.G. Chang

Of the emerging technologies for control of SO_2 and NO_x in flue gases, the spray-drying method has shown several economic and technical advantages over existing wet processes. To maximize the potential of a spray-drying desulfurization and denitrification system, reagents that effectively react with SO_2 and NO_x must be identified.

ACCOMPLISHMENTS DURING FY 1987

We have tested a number of compounds that are considered to have potential as spray-drying reagents in a bench-scale spray-drying system. A small spray dryer with a rotary atomizer to disperse the reagent solution into the hot flue gas was used. Simulated flue gas with about 500 ppm NO and about 2000 ppm SO_2 was heated and directed into the spray dryer. The test solution was fed into the atomizer. About 70% of the solid could be collected by a cyclone collector at the exit. A fraction of the gas leaving the system was directed into a chemiluminescent NO_x analyzer and a fluorescent SO_2 analyzer for measurement of the NO and SO_2 concentrations.

Two types of solutions were studied in the spray-drying system. One type of solution contained ferrous chelate complexes to bind NO and an alkaline compound to bind SO_2. The other type of solution contained oxidants to oxidize NO and SO_2 into nitrite/nitrate ion and sulfate ion. Runs were done at both room temperature at about 150°C. The gas flow rate was about 20 cfm.

EDTA, cysteine and cysteinylglycine were used as chelates in the ferrous chelate complex studies. Carbonate and/or bicarbonate salts were used as buffers. The chelates studied were chosen because they had worked well in bench-scale wet scrubbing systems. In the runs done with a gas inlet temperature of 25°C, cysteine had the highest removal of the chelates tested: 13%. EDTA and cysteinylglycine had lower removal rates. Some runs were done without oxygen, but no improvement in the NO removal rate was observed. The SO_2 removal was controlled by the amount of buffer present, and removal rates in excess of 90% could be achieved.

EDTA and cysteine were tested with a gas inlet temperature of about 150°C. As expected, the NO removal was less than that obtained at 25°C. Virtually no NO was removed with EDTA as a chelate, while NO removal was as high as 11% with cysteine as a chelate. Again, SO_2 removal in excess of 90% could be obtained. A test done by the Pittsburgh Energy Technology Center on ferrous cysteine in a similar system with a gas inlet temperature of 180°C obtained 24% NO removal and 96% SO_2 removal. From the results, it appears that ferrous chelate solutions are not well suited to spray-drying flue gas clean-up.

The second class of solutions studied, oxidants, had also showed promise in wet scrubbing NO_x and

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SO_2 removal systems. The oxidants studied include H_2O_2, $NaClO$, $NaClO_2$, $NaClO_3$, $NaClO_4$, $Ca(ClO)_2$, $(NH_4)_2S_2O_8$ and $NaIO_4$. Most of these compounds were tested with gas containing NO, but not SO_2, since SO_2 can be readily removed by alkaline solutions. Of these compounds, $NaClO_2$ and $NaClO$ proved to be the most promising. $NaClO$ was influenced by the gas temperature significantly, and could remove up to about 20% of the NO. $NaClO_2$ worked well at 25°C, removing up to 75% of the NO, but its efficiency decreased with increasing temperature. It could remove less than 10% of the NO at 150°C.

PLANNED ACTIVITIES FOR FY 1988

There are many other possible compounds that may be useful in spray-drying systems. We plan to continue our search to identify effective and inexpensive compounds or mixtures of compounds for use in commercial spray-drying systems for SO_2 and NO_x control.

Removal of NO_x and SO_2 from Flue Gas by Treatment with Peroxyacids*

D. Littlejohn and S.G. Chang

Cost-effective and efficient methods are needed to simultaneously remove SO_2 and NO_x from flue gas effluent from coal-fired power plants. Metal-chelate based systems for simultaneous desulfurization and denitrification of flue gas show promise, but are generally sensitive to the oxygen in the flue gas. Use of oxidizing compounds as scrubbing agents would avoid the problem of oxygen sensitivity. One class of oxidizing compounds, peroxyacids (peracids), have been found to be particularly effective in removing NO_x and SO_2 from simulated flue gas.

ACCOMPLISHMENTS DURING FY 1987

Peroxyacids can be formed by mixing concentrated (30-70%) hydrogen peroxide with concentrated acid. The general reaction is:

$$X-OH + H_2O_2 \rightleftharpoons X-OOH + H_2O$$

where an equilibrium exists between the peroxyacid and the acid. The peroxyacids which have been investigated so far are peroxysulfuric acid, peroxyformic acid and peroxyacetic acid. The ability of the peroxyacid solutions to remove NO and SO_2 from flue gas was studied in both a wet scrubbing system and a spray-drying system.

In the wet scrubbing system, the gas mixture containing NO and SO_2 was bubbled through a glass frit immersed in the peroxyacid solution. The gas mixture was then directed through a cold trap and to a chemiluminescent NO_x analyzer and a fluorescent SO_2 analyzer. The temperature of the scrubbing column containing the peroxyacid solution could be adjusted, if desired. NO concentrations of 360-550 ppm and SO_2 concentrations of 1400-2460 ppm were used in the experiments. A gas flow rate of 1 l/min was used with a scrubbing solution of 50 ml. The concentrations of the peroxyacids in the solution ranged from 1 to 4 M. The equilibrium constants for the acids differ and are temperature dependent. The temperature studied ranged from 25°C to about 55°C.

In all the wet scrubbing experiments where it was present, there was 100% removal of SO_2. Removal of NO was usually lower, although the removal of NO increased with increasing temperature. Runs done without SO_2 had better NO removal than runs done with NO. All three peroxyacids appeared to have similar abilities in NO and SO_2 removal. At 55°C, 90% NO removal and 100% SO_2 removal could be achieved.

In the spray-drying experiments, the gas mixture was heated to 110°C to 170°C before entering the chamber. The gas flow rate was about 600 l/min. The peroxyacid solution was fed into a rotary atomizer at a flow rate of 10 to 30 ml/min. The NO concentrations ranged from 550 to 850 ppm and the SO_2 concentrations ranged from 240 to 2740 ppm. The temperature of the gas leaving the spray-drying chamber ranged from 50°C to 95°C. In general, the amount of NO and SO_2 removed in spray-drying experiments were not as high as those achieved in the wet scrubbing experiments. The fraction of NO

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removed ranged from approximately .04 to .41 and the fraction of SO_2 removed ranged from approximately zero to 1.00. Higher scrubbing solution feed rates increased the fraction of NO and SO_2 removed. Higher spray-drying temperatures increased NO removal but decreased SO_2 removal. The optimum conditions have not been determined.

PLANNED ACTIVITIES FOR FY 1988

We plan to continue studies of peroxyacids as flue gas scrubbing agents. The chemistry of the removal process and the reaction products will be investigated. The use of additives to improve removal rates in the spray-drying system will be attempted.

Disulfate Ion as an Intermediate in the Oxidation of Bisulfite Ion by O_2*

D. Littlejohn, K.Y. Hu and S.G. Chang

Most methods of removing SO_2 from flue gas involve the interaction of the gas with aqueous solutions. The SO_2 will readily dissolve in an aqueous solution, where its charge state will depend on the pH of the solution. The oxidation of the dissolved SO_2 is influenced by a number of factors, which must be understood to treat the scrubbing solution and remove the dissolved sulfur oxyanions.

ACCOMPLISHMENTS DURING FY 1987

Bisulfite ion (HSO_3^-) is the predominant form of dissolved SO_2 in the range of pH 2 to 7. The reaction of dissolved O_2 with HSO_3^- was studied using a high-pressure, rapid mixing flow system and a Raman spectrometer. By pressurizing the reaction system, the dissolved oxygen concentration could be raised to a level where it could be observed by Raman spectrometry. The reaction was studied by either collecting a Raman spectrum of mixed reactants while they flowed through the cell, or by observing the behavior of a Raman line of one compound when the flow was stopped.

In the studies of this reaction, an intermediate in the reaction was observed. From its behavior, we assigned $S_2O_7^{2-}$ as the formula for the intermediate. The intermediate hydrolyzes to form sulfate and hydrogen ion:

$$S_2O_7^{2-} + H_2O \rightarrow 2H^+ + 2SO_4^{2-}$$

From the hydrolysis rate constant and reaction products, and from the Raman spectrum, the intermediate has been identified as disulfate ion.[1] Sodium disulfate salt was prepared[2] and its Raman spectrum and hydrolysis rate was compared with those of the intermediate. The Raman spectra are shown in Fig. 1. Spectrum A is that of disulfate ion at 25°C. Data were collected in selected regions only because of its limited lifetime. Spectrum B is of disulfate ion at O°C, where it is longer-lived. Spectrum C is the difference between freshly mixed and completed reacted $O_2 + HSO_3^-$. The two peaks at 1023 and 1055 cm^{-1} are due to HSO_3^-. The hydrolysis rate constant of the intermediate agrees very well with that of disulfate ion.[3]

PLANNED ACTIVITIES FOR FY 1988

The hydrolysis of disulfate ion is influenced by a number of metal cations.[3] We plan to study the influence of metal ions commonly found in scrubber

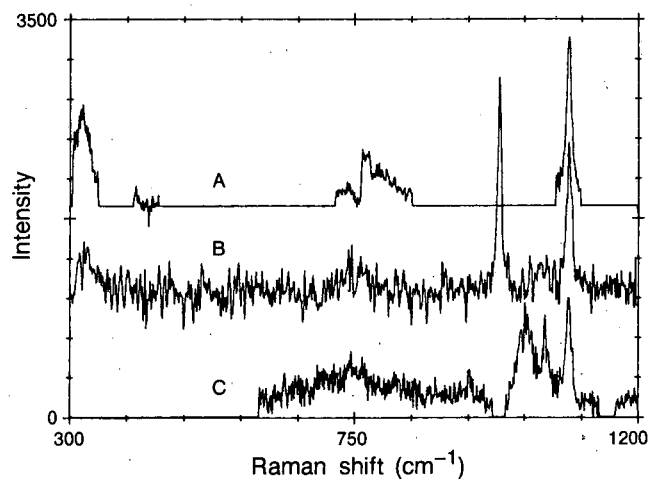

Figure 1. Raman spectra of A) disulfate ion at 25°C, B) disulfate ion at 0°C, and C) intermediate in reaction system. (XBL 8710-5923)

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systems on the $S_2O_7^{2-}$ hydrolysis rate. Little is known about the formation of disulfate ion in the $O_2 + HSO_3^-$ reaction system. It is desirable to understand the mechanism by which it is formed.

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A Study of the Solubilities of Nitrogen-Sulfur Compounds*

D. Littlejohn, A. Johnson and S.G. Chang

The nitrogen-sulfur compounds hydroxyimidodisulfate (HIDS), hydroxysulfamate (HSA), nitridotrisulfate (NTS), and imidodisulfate (IDS) are formed by reactions of nitrite ion (NO_2^-) with bisulfite ion (HSO_3^-) in acidic or neutral solutions. Appreciable amounts of NO_2^- and HSO_3^- can form in some scrubbing systems designed to remove SO_2 and NO_x from flue gas. The solubilities of these nitrogen-sulfur compounds are needed, so that methods for removing them from scrubbing liquors can be developed.

ACCOMPLISHMENTS DURING FY 1987

The potassium salts of the nitrogen-sulfur compounds are among the least soluble of those with common cations. The potassium salts were prepared by methods given in the literature.[1,2,3] Saturated solutions of the salts were prepared by adding excess salt to water in a controlled-temperature bath. After allowing sufficient time for saturation to occur, the concentrations of the dissolved salts were determined. Two analytical methods were used. In the first method, a measured volume of the saturated solution was mixed with a measured volume of a sodium sulfate solution of known concentration. A Raman spectrum of the mixed solution was obtained, and the original concentration of the nitrogen-sulfur compound was calculated from the Raman peak heights.[4]

*This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal Utilization Systems, U.S. Department of Energy under Contract No. DE-AC03-76SF00098 through the Pittsburg Energy Technology Center, Pittsburgh, PA.

In the second method, reference solutions of known concentrations were prepared for the nitrogen-sulfur compounds. Dilutions of the saturated solutions were prepared. For each compound, diluted samples and the reference solution were alternately injected into an ion chromatograph. The peak heights were then used to calculate the concentration of the saturated solution.[5]

Measurements were made on the potassium salts of HIDS, NTS and IDS. The measurements on IDS were complicated by the process:

$$IDS^{2-} \rightleftharpoons IDS^{3-} + H^+ \qquad K_{a3} = 3.3 \times 10^{-9}$$

More work needs to be done under controlled pH conditions to obtain accurate data. For HIDS, the solubility as a function of temperature can be described as:

$$\text{solubility (moles/liter)} = 0.0106T(°C) - .033$$

for a temperature range of 5 - 40°C. For NTS, the solubility equation is:

$$\text{solubility (moles/liter)} = 4.3 \times 10^{-4}\, T(°C) + 2.9 \times 10^{-3}$$

over a temperature range of 5 - 65°C.

PLANNED ACTIVITIES FOR FY 1988

We plan to continue making solubility measurements on these compounds. Solubility of the two charge states of IDS are needed, as well as the solubility of HSA. It would be useful to have solubility data on all the compounds above 50°C.

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COMBUSTION RESEARCH

Controlled Combustion*

P.R. Breber, N.J. Brown, J.A. Cavolowsky, D.W. Faris, K. Hom, D. Lucas, J.A. Maxson, A.K. Oppenheim, D.A. Rotman, R.F. Sawyer and H.E. Stewart

The goal of this project is to provide scientific background for the development of controlled combustion engines. Their practical attributes consist of: 1° minimization of formation of pollutants, 2° optimization of the tolerance to a wide variety of fuels, and 3° maximization of fuel economy. In order to attain this, combustion chambers, considered so far as solely sources of power, have to be transformed into controlled chemical reactors. In principle this involves a fundamental modification of the combustion process so that, instead of having to rely upon a solitary flame, a single connected zone separating the burnt gas from the unburnt medium, it is accomplished by a multitude of flame kernels generated by exothermic ignition centers which are appropriately distributed throughout the working substance.[2,10,14] The best way to realize this is by the use of jets, capable of impregnating the combustible charge with controllable sets of ignition sources. Thus, the primary objective of experimental investigations was the exploration of the properties of pulsed jets, or puffs, of plasma, hot gas (flames), and liquid fuel (sprays), whereas, concomitantly, the fluid mechanical and thermochemical features of ignition and turbulent combustion fields and jets were at the focus of theoretical studies.

ACCOMPLISHMENTS DURING FY 1987

Pulsed Plasma Jets

Experimental investigation of the thermochemical and fluid mechanical properties of pulsed plasma jets was carried out by the use of, respectively, the molecular beam mass spectroscopy (MBMS) and the ultra-high frequency (~ MHz) schlieren cinematography. Last year, we developed a technique to calibrate the mass spectrometer for a quantitative determination of species concentrations. On this basis we measured concentration histories of such radicals as O, N and NO, produced by plasma jet igniters in nitrogen and air.[3] This led to the establishment of the MBMS technique for concentration measurements in combustible mixtures, applicable, in particular, to active radicals, such as CH_3, O, H, and OH, in lean hydrocarbon-air mixtures - a subject currently under study.[13] At the same time, the schlieren records we obtained revealed the salient fluid mechanical features of pulsed plasma jets.[14] They demonstrated, in particular, that the jets can be wholly subsonic or embody a supersonic core. The former was found to provide a greater depth of penetration, indicating the advantage of unrestricted opening at the exit of the plasma cavity. Moreover, physical reasons for the impressive effectiveness of the jets in entraining the surrounding atmosphere and mixing were brought out by direct experimental observations.[12] This was confirmed by MBMS measurements,[3,13] providing a rationale for the application of pulsed jets as igniters of extremely lean mixtures.

Liquid Fuel Strays

Evaporation and deformation over liquid fuel droplets at near- and super-critical conditions that are typical of low heat rejection diesel engines[1,7] was explored. Taken under particular scrutiny in this connection were conditions at a stagnation point. In order to elucidate the mechanism of the process, we introduced a number of simplifying assumptions concerning the physical properties of the substance, and expressed the energy and species conservation principles for the transient state under study in terms of transport equations for vorticity and temperature in both liquid and gas phase. These were solved simultaneously, subject to appropriate boundary conditions, to yield profiles of vorticity, temperature, and species concentrations, as well as the regression rate of the interface between the fuel and the gas stream. On this basis computations were performed for octane as a representative fuel. Its initial temperature was taken as 300°K, while the environment was assumed to be at 2300°K. Two cases were examined, the near-critical when the pressure was 0.166 MPa below the critical value of 2.526 MPa,

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and the super-critical corresponding to twice this pressure. The results demonstrated a distinct superiority of the latter in regression rate as well as in penetration depth, expressed in terms of the fuel concentration profiles.

Modeling Studies

The most significant progress in numerical techniques we developed was in the extension of the random vortex method to flow fields in enclosures via the zero Mach number model.[5,6,8,9,11] The most prominent result of these studies is the establishment of the fluid mechanical properties of flame fronts and the evaluation of their consequences in the case of flames propagating in enclosures, such as the cylinder-piston system of an engine. These are as follows: 1° advection at the local velocity of the unburnt medium, 2° self-advancement at a normal burning speed, 3° potential source due to exothermicity, 4° source of vorticity due to local baroclinic action. The first two are purely kinematic in nature, while the last two are dynamic, producing a feedback effect upon the flow field. All this applies irrespectively whether the flame is laminar or turbulent. The only difference between the two is that the normal burning speed, playing the role of an eigenvalue of the system, is, for the former, a function of the flame structure and geometry, while for the latter it is a property of the whole field. On this basis we analyzed flames propagating in containers of constant as well as variable volume, the latter simulating the piston-cylinder enclosure of an engine.[5,6] Our results demonstrated that some well-known combustion instabilities, associated with a significant distortion in flame shape, that hitherto were considered to be of acoustic origin, are basically fluid mechanical in nature.[9] Modeling of the combustion process in an engine yielded simulated pressure transducer records that were in good agreement with actual measurements.[5] Thus proper background has been laid down for the examination of the fluid mechanical consequence of some control measures, such as the substitution of a singular flame front traversing the charge, a solitary flame, by a multitude of flame kernels generated by exothermic centers that are produced by ignition jets. The igniters we developed for this purpose are described by Figs. 1 and 2. The first presents our design of a plasma jet igniter. Its prominent feature is the hollow electrode providing a duct for the introduction of proper feedstock into the cavity. The second embodies also a hollow electrode; in this case it is for the introduction of additional fuel to establish a significantly richer fuel/air mixture in the igniter cavity than that of the charge in the

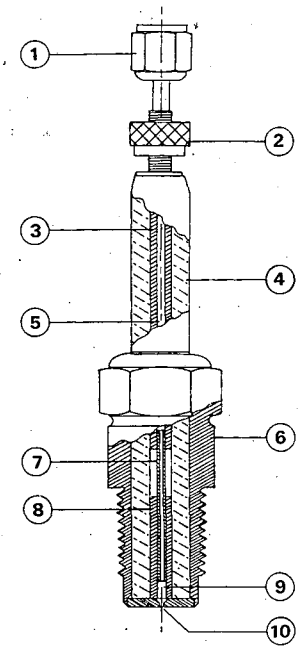

Figure 1. Plasma jet igniter; 1-tube fitting, 2-high voltage terminal, 3-steel tube, 4-insulator, 5-feedstock passage, 6-plug body, 7-nickel tube, 8-quartz tube, 9-plasma chamber, 10-discharge port. (XBL 881-302)

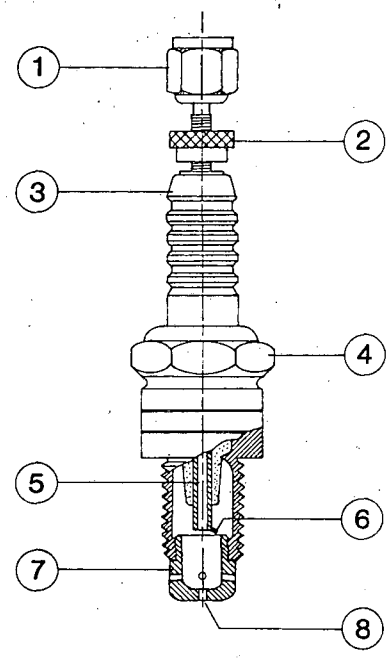

Figure 2. Flame, or hot gas, jet igniter; 1-tube fitting, 2-high voltage terminal, 3-insulator, 4-plug body, 5-nickel tube, 6-electrode, 7-injector tip, 8-discharge port. (XBL 881-303)

cylinder. The jet is thus full of hydrocarbon radicals to act as multiple ignition sources of an essentially lean working substance, providing thus the essential service for the transformation of the combustion chamber into a controllable chemical reactor, as pointed out at the outset.

PLANNED ACTIVITIES FOR FY 1988

In continuing our research on the scientific background and means for the development of controlled combustion engines, we plan to conduct a three-phase program of work.

1. Study the fundamental features of flame, or hot gas, jet ignition in a constant volume vessel using high-speed schlieren cinematography.
2. Test the performance of flame jet igniters under the influence of product recirculation, using a variable compression (C.F.R.) engine.
3. Investigate the atomization, evaporation, mixing, and inflammation of sprays produced by ultra-high pressure ($\sim$ kilobar) fuel injectors, using the shock tube apparatus we developed for this purpose.

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Smoke Emission Measurements from Medium Scale Experiments*

R.B. Williamson, R. Dod, F.W. Mowrer†, N.J. Brown, and T. Novakov

Knowledge of the quantity and character of the smoke emitted by fires occurring in the aftermath of a post nuclear exchange is crucial for predicting its climatic impact. Sooting is controlled by a complex interplay between chemical kinetics and fluid mechanics. Relative to our understanding of elementary reactions of small species, the understanding of the chemistry of larger species (soot precursors and soot) is in a very primitive stage. It is not possible to predict the soot quantity and character from our current understanding of the chemistry. Considerable problems of scale are also associated with identifying crucial heat transfer and turbulence parameters. The performance of smoke quantification and characterization measurements over a range of scales will make positive and important contributions to this most difficult and significant problem. The measurements should be accompanied by careful documentation of combustion conditions to enable researchers ultimately to employ the results obtained in controlled laboratory situations to extrapolate to conditions believed important in various post-nuclear fire scenarios.

To help quantify the smoke which might be generated following the use of nuclear weapons, and perhaps cause "Nuclear Winter," a series of medium-scale fire experiments with representative urban fuels, such as wood, asphalt roofing and liquid petroleum, has been conducted here at LBL. These experiments have been conducted under both well ventilated and underventilated conditions, and during each experiment the mass of smoke was determined by sampling the aerosol particulate in the exhaust duct which captured all the effluent from the burning material. The rate-of-heat-release (RHR) was measured by oxygen depletion calorimetry (ODC). Sampling probes were inserted through the wall of the duct and were designed to provide isokinetic sampling of the flowing smoke and combustion products. The direct measurement of the smoke particulates and their characterization is one of the unique features of this research program.

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†University of Maryland, Dept. of Fire Protection Engineering, College Park, MD 20742

ACCOMPLISHMENTS DURING FY 1987

During FY 1986, 13 experiments were conducted using softwood (both solid wood and plywood) and asphalt roofing shingles. As shown in Fig. 1, the smoke emission factors measured for burning wood under well ventilated conditions were in the range of 0.1 to 0.3 percent, but under limited conditions this increased an order of magnitude to the 1 to 3 percent range. The smoke emission factors measured for asphalt under well ventilated conditions are again an order of magnitude higher, in the 14 percent range. The implications of these measurements, in the context of Nuclear Winter, center around three aspects of the measurements. First, there is a substantial effect of ventilation on the smoke production from burning wood; it is significant that the smoke emission factors measured under limited ventilation conditions were more than an order of magnitude higher than those measured in well ventilated conditions. Wood is one of the major building and furnishing materials used in the United States, and it is reasonable to assume that large quantities of wood will burn under both limited and unlimited ventilation conditions in the post nuclear environment. A second aspect of the measurements is that the "medium scale" well ventilated wood experiments produced several orders of magnitude more black carbon than had previously been reported by bench scale experiments. It is the black carbon particles which absorb sunlight and produce the "Nuclear Winter" effects. A third aspect of the measurements is that the smoke emission factors found for asphalt roofing shingles, a total of almost 14 percent with 90 percent being black carbon, may have a significant impact on urban smoke products in the nuclear environment. These results have been presented at the Second International Symposium on Carbonaceous Particles in the Atmosphere, October 5-8, 1987, Lawrence Berkeley Laboratory, University of California, Berkeley, and are described in detail in References 1 and 2.

During FY 1987, the exploration of the smoke production of liquid petroleum, which represents one of the major fuel sources in the post nuclear environment, was added to our program. Medium scale experiments with No. 2 fuel oil have been conducted under both well ventilated and limited ventilated conditions. The smoke emission factors in the 8 to 9 percent range have been measured from 400 to 800 KW for well ventilated fires. The results of the limited ventilation experiments have not been reduced at this writing, but their emission factors appeared to be greater. The average particle emissions factors for all fuels types are shown in Fig. 1.

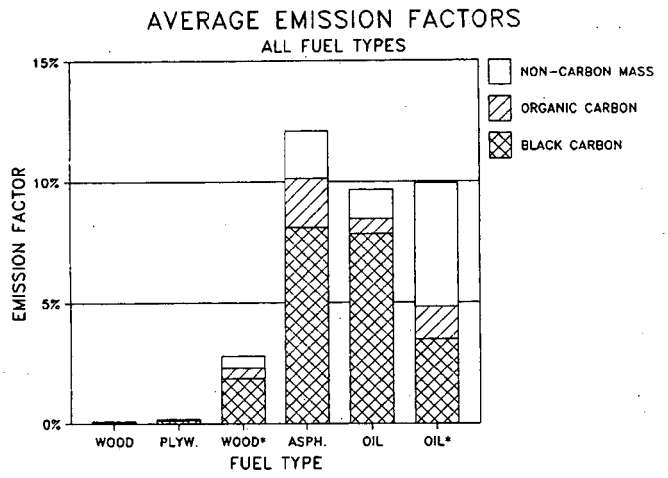

Figure 1. Histogram of the Smoke Emission Factors Measured for Various Fuels Burning under well ventilated conditions and limited ventilation conditions, marked with a *. (XBL 883-807)

PLANNED ACTIVITIES FOR FY 1988

A continuation of the medium scale experiments with increasing rates of heat release under various ventilation conditions in order to evaluate the effects of scaling. The study of scaling will be emphasized and ways of correlating the findings from these medium and large scale experiments will be explored.

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Combustion Chemistry*

N.J. Brown, R.J. Martin, and M. Longuemare

Combustion processes are governed by chemical kinetics, energy transfer, transport, and fluid mechanics, and the complex interactions among these. Understanding chemical kinetics and energy transfer offers the possibility of better understanding combustion so that it can be controlled to achieve decreased levels of pollutants and better efficiencies. In all chemical changes, the pathways for energy movement are determining factors. Competition among these pathways, including energy dissipation, determine product yields, product state distributions, and the rate at which reaction proceeds. This competition is influential in flames, explosions and shock waves. Advances of theories of reactivity have important impacts on our understanding of the chemistry affecting the emissions of pollutant species, rates of heat release during combustion, and the growth rates of undesirable combustion phenomena. The first portion of our research is concerned with understanding reactivity and energy transfer processes at the state-to-state level to determine rate-controlling factors.

The second portion of our research is concerned with understanding the combustion chemistry of nitrogenous pollutants, and is currently focussed upon nitrous oxide chemistry. Nitrous oxide is the principal source of stratospheric nitric oxide which is a major scavenger of stratospheric ozone. Nitrous oxide is also a greenhouse gas, and its residence time in the atmosphere is approximately 150 years. Its concentration in the atmosphere is increasing by 0.2% per year, and combustion is a major contributor to the budget. The factors which control N_2O

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emissions are not well understood so that it is not possible to inventory accurately anthropogenic sources other than by exhaustive source measurements. Furthermore, it is not possible to design cost-effective control strategies or to predict the efficacy of current NO_x techniques for N_2O reduction unless a more fundamental understanding of N_2O combustion chemistry is acquired.

ACCOMPLISHMENTS DURING FY 1987

Energy transfer in the coplanar, rigid rotor $H_2 + H_2$ system and its isotopic analogues (H_2 + HD and HD + HD) was studied with the method of classical functional sensitivity analysis. This was a collaborative research effort[1] with Herschel Rabitz and Richard Judson of Princeton University. Sensitivity Analysis is a general approach to understanding the relationship between the potential energy surface and a set of observables. The functional sensitivities measure the response of an observable to arbitrary variations of the potential at some point in configuration space.

The potential energy surface used for the H_4 system was determined by Silver and Brown[2], and this was expanded in a complete set of angular functions of the form $Vm_1m_2^{(R)} \cos(m_1Q_1+m_2Q_2)$. The sensitivities for each observable were also expanded in the same set of angular functions used for the potential as shown in Fig. 1, and this enabled us to measure the importance of individual terms in the potential. Trajectory sensitivities were calculated, and then each observable sensitivity for individual trajectories was calculated using the functional chain rule. Observable sensitivities for an ensemble were determined by ensemble averaging the trajectory values, and this required approximately 1000 trajectories. Calculations are computationally very intensive. We have found that sensitivity analysis for problems of importance in molecular physics provides new and exciting information, and that this has the potential for really challenging some of the more traditional ideas about collisions.

Five major conclusions were reached as a result of this study:

(1) Small magnitude, high order terms in the potential (as measured by an expansion in a complete set of angular functions) can affect the final energy distribution in important ways.

(2) Particular terms in the potential can influence individual observables quite differently.

(3) For the isotopic combinations examined (with the possible exception (HD +HD), rotation-rotation and rotation-translation energy transfer process are approximately separable in the sense that varying a particular term in the potential will only affect energy transfer between a single pair of degrees of freedom.

(4) Rotational-translational energy transfer processes are much more sensitive to the potential than are the rotational-rotational

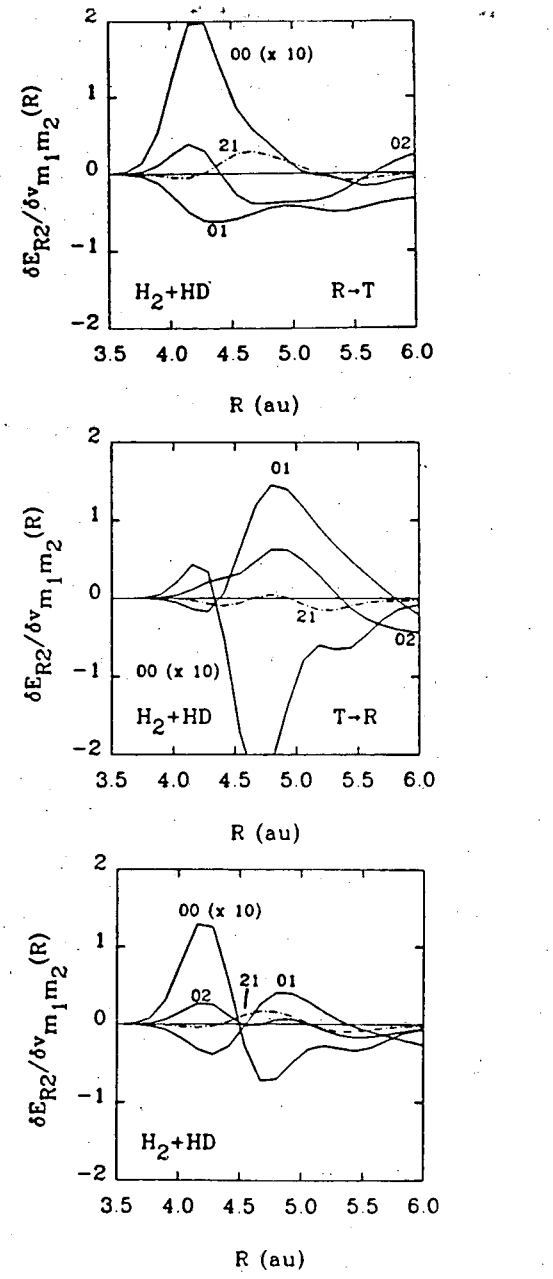

Figure 1. The largest sensitivity functions for the HD molecule for the case H_2(j=1) and HD(j=3). The values of all curves have been multiplied by 1000 and units are au^{-2}. The first index is the value of m1 and the second represents m2. (XBL 882-609)

ones, and this result is partially due to the use of classical mechanics. A consequence of the rotational translational dominance is that the effect of altering a term in the potential responsible for transferring energy between translation and rotation of one molecule is not very dependent on the identity of (HD or H_2) of the other molecule.

(5) The influence of the potential on the energy transfer into or out of each of a pair of identical molecules is quite sensitive to the initial rotational energy of the molecules.

Another problem that was investigated was rotational relaxation of HD. This study was performed to model the experiments of Chandler and Farrow[3] (CF) of Sandia National Laboratory. In these studies HD molecules were excited to v = 1 and a specific J state such that $J \leq 6$, and these collided with HD molecules in a thermal distribution at 298K. The rate coefficients required to determine the relaxation time of the excited state distribution were determined. This study was a molecular dynamics one which employed the Silver/Brown surface B. Some of the assumptions regarding the dynamics that (CF) employed in the analysis of data were investigated in our theoretical studies. Average energy transfer quantities per collision, correlation coefficients, and rate coefficients were computed. Particular attention was paid to angular momentum exchange among the three types and to whether or not there was an appreciable average change in the z component of angular momentum. Because there was more rotational-translational exchange than rotational-rotational exchange, the correlation between j_i (where i = 1 or 2) and orbital angular momentum was stronger than j_1 or j_2. The vibrational degrees of freedom of the two molecules were highly coupled. In our study changes of j of more than 2 angular momentum units were quite rare, and the corresponding rate coefficients for these transitions agreed satisfactorily with the values of CF.

Modeling calculations have been performed[4] to illustrate the effect of using five commonly accepted data bases of thermochemical properties on predictions of temporal species profiles. The thermochemical properties are those used for the determination of equilibrium constants employed in the calculation of reverse rate coefficients for a chemical mechanism where forward rate coefficients are specified. The modeling study was performed for hydrogen/oxygen/argon/nitrogen-compound mixtures where the nitrogen compound was either NO or NH_3. The mixtures reacted isothermally at 1600 K and isobarically at 1 atmosphere, and a single kinetic mechanism for which forward rate coefficients were specified was used throughout. Mixtures of equivalence ratios of 0.625, 1.0 and 1.6 were considered. Modifications in sources of thermodynamic data have been substantial since 1971 for some species. Among the data bases, thermochemical properties varied greatly for the species NH, NH_2, NNH, and HO_2, and those for other species important in the mechanism had variations of less than 10 percent. The single most important result of our study is that the thermochemical property variations for NH, NH_2, NNH and HO_2 among the data bases have substantial effects upon the temporal species profiles for nitrogenous species. This is most pronounced for rich combustion, and varies directly with equivalence ratio. Use of different data bases had little effect on the H/O species profiles. Radical species profiles (with the exception of HO_2) tend to be influenced strongly by their own thermochemical properties. Computed profiles also were shown to be independent of algorithm (HCT or CHEMKIN) and thermodynamic property fitting procedure between 1000 and 2000 K.

Nitrous oxide production and destruction were investigated in laminar, one dimensional atmospheric pressure flames[5]. The experimental variables were bulk flow rate, equivalence ratio, nitrogen compound type, nitrogen concentration, and fuel type. Radial and axial temperature and composition profiles were measured. Nitrous oxide is formed in lean CH_4/air and H_2/air flames doped with N_2, NO, N_2O, and NH_3, but it does not survive into the post flame zone. Nitrous oxide concentration was found to depend inversely upon final flame temperature and equivalence ratio and directly upon nitrogen compound concentration. In decreasing order of observance of early N_2O, the four dopants can be ranked: N_2O, NH_3, NO, and N_2. Nitrous oxide profiles were similar in both CH_4 and H_2 flames. Radial profile measurements showed increased amounts of N_2O existing near the burner edge. Modelling calculations were also performed for the H_2 flames with the four nitrogen dopants. Comparison between calculated NO and N_2O profiles and those measured in the flame showed that our understanding of nitrogen combustion chemistry is still deficient.

PLANNED ACTIVITIES FOR FY 1988

Research in both of these areas will continue.

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Combustion Fluid Mechanics*

R.K. Cheng, I.G. Shepherd, and L. Talbot

Although it is well known that fluid mechanical turbulence increases the overall combustion reaction rate, the exact relationship between turbulence intensity and mean burning rate remains a major unresolved issue in fundamental turbulent combustion research. The overall goal of this program is to gain a better physical understanding of the controlling turbulence-combustion interaction processes through detailed study of the complex turbulent combustion flowfields in simplified laboratory scale burners. By the use of laser diagnostic techniques which measure scalar and velocity fluctuations and cross-correlations, the detailed statistical data are obtained for comparison with predictions of theoretical models and for determining burning rates.

ACCOMPLISHMENTS DURING FY 1987

In FY 1987 we have developed a new experimental procedure and method of analysis to deduce the turbulent burning rate $\overline{w}$[1]. This study is motivated by the fact that to date, the most convenient means to express the increase in burning rate is by the use of the turbulent burning speed, S_T. The large uncertainties associated with determining S_T using the conventional flame orientation method have been reported in the literature. In many cases the results have been shown to be rather meaningless[2]. Consequently, reliable S_T data has only been obtained in configurations specially designed to reduce the uncertainties but not in practical burners which have complex flame geometries. Therefore, an alternate means to determine S_T which is independent of flame geometry is highly desirable.

Our analysis is based on capitalizing recent theoretical works of Bray and co-investigators. Central to their theory is a model of the reaction rate which is expressed in terms of the the mean flame crossing frequencies, ν. The most significant feature of the crossing frequency concept is that ν can be measured directly in experiments using simple laser techniques. Their latest model (Bray, Champion and Libby (BCL)[3], indicates a convenient means to investigate the functional relation between S_T and $\overline{w}$. This important aspect of premixed turbulent flame propagation has remained largely unexplored by experiment. The significance for theoretical developments is that the relationship between $\overline{w}$ and S_T could be used in validating the model and obtaining new closure techniques for predicting the burning rate.

The model treats the turbulent flame region as consisting of a thin wrinkled fluctuating flame interface which separates the the unburned reactants from the burned products. Under the fast chemistry assumption, this scalar quantities can be represented by a single progress variable, c. The second and third order turbulent transport terms can then be expressed in terms of c and the conditioned velocities in the reactants and products zones U_r,U_p. The reaction rate $\overline{w}$ is expressed by a simple equation $\overline{w}(x) = w_f(x)\nu(x)$ where ν is the number of flame crossings per unit time and w_f is the mean rate of creation of products by each crossing. By further assuming that the flame sheet consists of laminar

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flamelets, BCL [3] models w_f as $w_f = \rho_r S_L / U_n$ such that

$$\overline{w} = \frac{\rho_r S_L \nu(x)}{U_n(x)}$$

where S_L is the laminar burning speed of the flamelet and U_n is the mean convection speed of the flamelet with respect to the laboratory frame.

The most significant feature of this model is its simple relationship to the turbulent burning speed. For a one dimensional flame, it can be demonstrated that the integration of the reaction rate from $x = 0 \rightarrow \infty$ determines the turbulent burning rate. By analogy to the laminar burning rate $\rho_r S_L$, the turbulent burning rate is $\rho_r S_T$. Therefore,

$$\int_0^\infty \overline{w}\, dx = \rho_r S_L \overline{W} = \rho_r S_T$$

where

$$\overline{W} \equiv \int_0^\infty \frac{\nu(x)}{U_n(x)}\, dx$$

$\overline{W}$ is the ratio between the turbulent burning rate and the laminar burning rate and is identical to the turbulent/laminar burning speed ratio S_T/S_L.

To verify Equation (1), experimental measurements of $\overline{w}$ in the two configurations were carried-out. The configurations are 1) rod-stabilized oblique v-flames and 2) large Bunsen conical flames. The flame crossing frequencies ν are measured by monitoring the Mie scattering from a silicone aerosol introduced into the reactant stream. The technique is based on the principle that the oil droplets evaporate and burn at the thin flame front. Since our analysis involves integrating the experimental data obtained through the flame brush, the choice of traverse trajectories is significant. In the past, data have been obtained along fixed vertical or transverse axes in laboratory coordinates. This was due mainly to limitations in the traversing mechanism for the diagnostic probe. A more logical choice is to measure along the mean flowlines i.e. the Lagrangian lines.

Since our setup consists of a computer controlled data acquisition system interfaced with a three dimensional traverse laser table and a two component laser Doppler anemometry (LDA) system, it is possible to trace automatically a flowline as specified by the local two dimensional unconditioned velocity vector. Figure 1 shows examples of the mean flowlines measured in the v-flame and in the conical flame. From a starting point x_0 and y_0 within the reactants, the system determines the next measurement position by measuring and computing the mean velocity components $\overline{U}$ and $\overline{V}$, then moves the LDA probe by a fixed increment in the direction of the velocity vector.

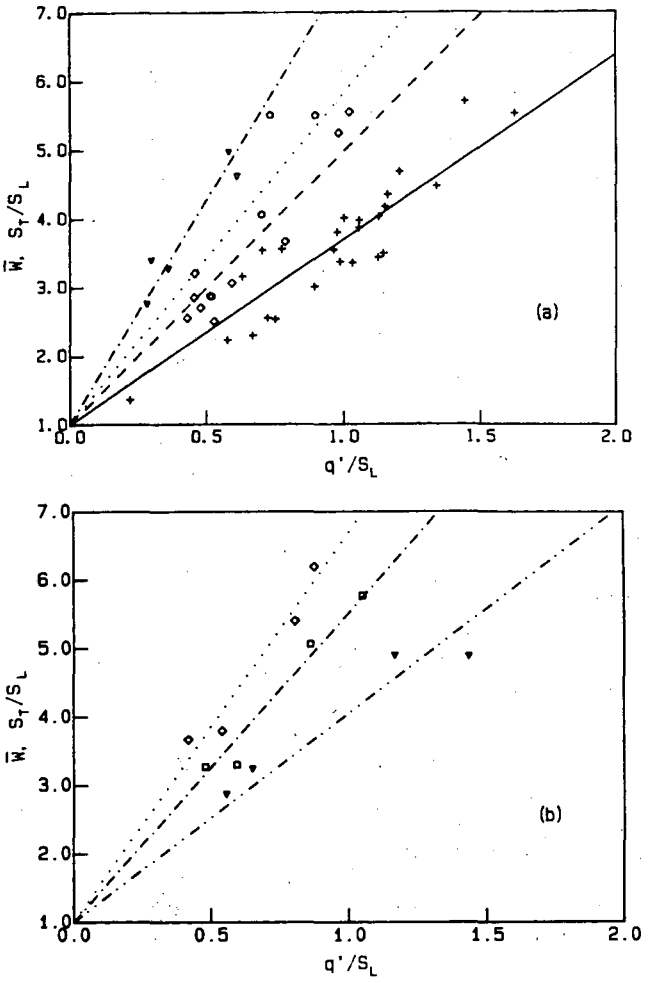

Figure 1. Typical 2D mean Lagrangian flowlines used for flame traverse and $\overline{c}$ = 0.1 and 0.9 contours for v-flame and conical flame. (XBL 8712-5389)

There are several laser diagnostics techniques suitable for measuring the convection speed of the flame fronts, U_n. However, these techniques are not very convenient for collecting large amount of data for statistical analysis. Since previous studies have shown that U_n in both of the configurations are very close to the mean flow velocity, for our analysis we have used the conditioned velocity in the reactants.

Measurements were made in five v-flames and four conical flames using methane/air mixture with various equivalence ratios and incident turbulent intensities. For each flame, two flowlines initially at

y_0 = 10 and 20 mm from the centerline were traced through the flame brush. In addition, traverses along the centerlines of the conical flame were also made. The values of $\overline{W}$ were determined by integrating ν/U_τ along these flowlines. Since $\overline{W} = S_T/S_L$, they can be compared directly on the conventional S_T/S_L versus q'/S_L plane where q' is the turbulent kinetic energy of the incident flow. Shown in Fig. 2(a) is the correlation of $\overline{W}$ in the v-flames with q'. Also shown are the ratios S_T/S_L in CH_4 / air stagnation point stabilized flames under similar flow conditions. The results determined previously for ethylene/air v-flames using the flame orientation method are also plotted for comparison. The various sets of results are fitted linearly by a least mean square. It is apparent that our $\overline{W}$ results are in good agreement with those of the stagnation point flames. They are also consistent with those deduced by the flame orientation method. However, the present analysis is a significant improvement since the uncertainty based on integrations is substantially reduced.

The result obtained in the conical flames are shown in Fig. 2(b). In contrast to the v-flame results, the conical flame results show a consistent trend of increasing $\overline{W}$ towards the flame tip region. This is better illustrated by fitting separately the results obtained on the centerline, at y_0 = 10.0 and 20.0 mm. The profiles with y_0 = 20.0 mm are within the oblique flame zone and closest to the burner rim. The most significant aspect of the conical flame results is that prior to this study, the burning speed along the centerline has not been reported because as mentioned earlier the flame orientation method implies that the turbulent burning speed is equal to the approach flow velocity. By using the flame crossing frequency method, we have demonstrated that the turbulent burning speed can be determined with confidence in more complex flame geometries.

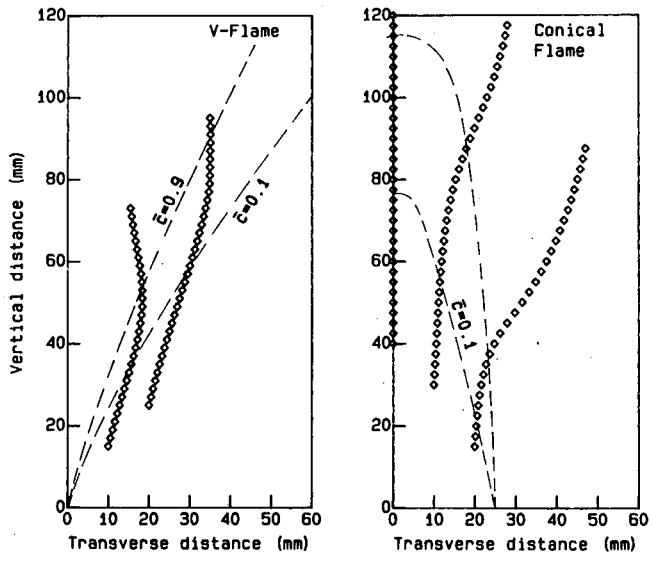

Figure 2. Correlation of the turbulent burning rate $\overline{w}$ with incident turbulence intensities (a) comparison of the results in v-flames (broken lines) and stagnation flow stabilized flames (solid line), (b) Comparison of $\overline{w}$ obtained in the conical flames along flowlines originating at y_0 = 20, 10, and centerline. (XBL 8712-5390)

In addition to our experimental works, progress has also been made in our numerical study of premixed turbulent flames using the vortex dynamic technique. As reported in FY 1986, the numerical work complements the experimental studies and assists in determining the controlling process for turbulent productions due to combustion. In FY 1987, we have explored the means to improve the algorithm for describing the movements of the flame interface. The technique used in the previous study assumes that the flame fronts advance normal to the local flame tangent at the laminar burning speed. This technique cannot consider the effects of flame curvature on local burning speed and does not permit the flame interface to form into flame cusps. A new flame movement algorithm develop by Prof. J. Sethian for vortex dynamic simulations of premixed turbulent flames is capable of overcoming these limitations. This algorithm is being incorporated into our numerical program for the v-flames.

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The method of determining the turbulent burning speed for premixed turbulent flames will be used to conduct a parametric study to correlate S_T with turbulence of various intensities and length scales. The experiments will be carried-out in conical flames, stagnation point stabilized flames, and in open and partially enclosed v-flames. One of the most interesting implication of the relationship between the reaction rate and turbulent burning speed is that the turbulent/laminar burning speed ratio is also directly proportional to the increase in flame area due to turbulence. In FY 1988 we plan to conduct a tomographic study of the flame front dynamics and flame geometries using a video camera system interfaced with the image analysis system. The shape and size of the flame wrinkles and the flame area in two-dimension can be determined and compared with theoretical predictions.

The vortex dynamics simulation of the v-flame will be extended to include the new algorithm which

considers the variation of the flame speed due to curvature. The evolution of the shape of the flame interface predicted by this model will be compared with those shown by tomography. Also deduced from the numerical results are the conditioned velocity statistics which can be compared with previously obtained experimental data.

The study of non-premixed (diffusion) turbulent flame will be initiated. Our approach is to investigate non-premixed turbulent flames at moderate to low Reynolds numbers. All of the diagnostic techniques and associated data reduction methods can be used for this study. A turbulent jet flame burner with adjustable co-flowing air will be constructed.

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Photochemical Conversion of Solar Energy by Microbial Systems*

L. Packer, R.J. Mehlhorn, I.V. Fry, J.J. Maguire, S. Spath, K. Tsujimoto†, W. Nitchmann, E. Hrabeta-Robinson, M. Huflejt, J. Hrabeta, M. Semadini and C. Reveron‡

The Membrane Bioenergetics group is currently investigating biological oxidations and bioenergetics in three areas: i) cyanobacteria, ii) bacteriorhodopsin (bR), and iii) bacterial succinate dehydrogenase (SDH). An overview of our most recent and novel results is presented, with the pertinent references to our publications.

ACCOMPLISHMENTS DURING FY 1987

Cyanobacteria

Cyanobacteria are a versatile species whose biochemistry readily adapts to changes in environmental conditions. Stress conditions (salinity) were used as a probe to investigate these adaptive processes on both functional and structural-compositional levels. Magnetic resonance spectroscopy (NMR and EPR) proved to be useful non-invasive tools for monitoring adaptive changes in whole cells of *Synechococcus* 6311 after a transition from low (0.01 M) to high NaCl (0.5M).

Structural-compositional Studies

During the past year we have clarified the temporal sequence of responses accompanying salt stress and adaptation. Using ^{23}Na- and ^{31}P-NMR analysis it was shown that the rapid penetration of Na^+ resulted in the disruption of ATP synthesis. However, during adaptation, the pattern of ^{31}P metabolites was similar to control cells, except that they produced more (and more intense) peaks in the monoester sugar phosphate region. The gross effects of stress were manifest as decreases in growth rate, photosynthesis, increases in respiration, sodium proton exchange activity and glycogen content. Examination of cells during various stages of the stress and adaptation process using flow cytometry, thin section and freeze fracture electron microscopy, showed that one minute after salt shock, virtually all the intracellular granules disappeared, the density of the cytoplasm decreased and the appearance of DNA material was changed. Four hours after salt exposure there was a reappearance of glycogen (preferentially between the cytoplasmic membrane and the thalykoid membrane) and other granules. At this time the photosynthetic oxygen evolution rate began to recover and respiratory activity was already substantially elevated. A decrease in the total number of membrane particles was observed at 4 hours with a shift from small to large particle size. After 24 hours the particles increased in total number and the large sized particles predominated. This pattern was not observed in the cytoplasmic membrane of control cells and it suggests synthesis of new membrane proteins in agreement with the known increases in cytochrome oxidase and sodium proton exchange activity[1-3].

Functional Studies

Concomitant with the structural-compositional changes, respiratory adaptations were also evident. *De novo* synthesis and levels of the terminal electron acceptor, cytochrome *c* oxidase, were investigated using purified cytoplasmic membranes which exhibited low temperature EPR spectra in the $g = 2.08$ region. This characteristic copper signal arose from a center in an environment identical to the aa_3-type cytochrome *c* oxidases reported in mammalian, yeast and bacterial systems. Membrane purification procedures demonstrated that the oxidase was present in the cytoplasmic membrane at ten times the level present in the thylakoid membrane. The copper was demonstrated to be fully redox active by its reducibility with physiological electron donors[4,5].

Applications of Cyanobacterial Productivity

The feasibility of using photosynthetic microalgae as a component in a Controlled Ecological Life Support Systems (CELSS), with particular emphasis

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†Visiting associate professor, on leave from the University of Electro-communication, Chofu, Tokyo.

‡LBL/JSU/AGMEF Summer Faculty Programs.

on the manipulation of biomass components was addressed. Using factors which retard growth but not photosynthesis, the partitioning of photosynthate may be directed towards carbohydrate and away from protein synthesis. Cold shock of dense cultures increased the glycogen content from 1% to 35% dry weight, and presents a technique to change the protein/carbohydrate ratio to a nutritionally acceptable level[6].

Antioxidative Effects of Organic Ge

The effects of an organic germanium sesquioxide (Ge-132) complex on the biochemistry of the cell was determined. The experimental approach was to assess concentration dependent toxic effects, by growth curve analysis, to monitor the bioenergetic impact of Ge-132 on photosynthesis and respiration, and to determine the assimilation and cellular distribution of germanium.

Bacteriorhodopsin

Bacteriorhodopsin (bR) is a protein in the purple membrane regions of the cytoplasmic membrane of *Halobacterium halobium* which translocates protons upon light absorption, and is one of the simplest known biological pumps. To elucidate the molecular mechanism, the role of amino-acid residues in the photocycle, and how this relates to cation binding was investigated using chemical modification of carboxyl and tyrosine residues. The proton pumping activity was affected only in the case of iodinated tyrosine samples. Modification of carboxyl residues influenced the time course of the photocyle but did not change the number of pumped protons per photocycle and the R-values evaluated. The effects of cation binding to chemically modified carboxyl groups were studied. Visible and EPR spectroscopy showed that two cations bind on the surface and at least one site is located in the protein interior. The fractional conversion of the blue to purple species by cation titration, heat treatments (cation release) and Mn binding showed that internal cross-linking or tempamine labeling disrupts cooperativity and weakens the cation binding site. Thus, internal and external carboxyl residues, and structural mobility within bR are essential to formation of the cation binding site. White membranes from the JW-5 strains reconstituted with all-trans retinal (WMrec) were also found to form the blue species. In this case, titration studies showed that up to 100 divalent cations bind to reform purple species. WMrec shows less cooperative association than in native bR, however, heat treatment studies suggest a greater stabilizing effect of cations on the structure of the WMrec than bR. Hence, negatively charged lipids in WMrec regulate cation binding[7-11].

Succinate Dehydrogenase (SDH)

An understanding of the mechanism, structure and assembly of complex metalloenzymes is important in understanding the complex interactions that exist between the transport of electrons through protein complexes and the relationship between protein electron transport and biological energy transduction. Little is known about the structure and the assembly-functional integrity of complex membrane proteins. In order to address this question mutants of *Bacillus subtilis* with specific lesions in the succinate dehydrogenase redox complex were analyzed using gene mapping, low temperature EPR and molecular weight analysis of native and truncated fragments of the protein subunits. The following new information about the assembly of one of the covalently bound iron sulfur clusters, cluster S-2, was determined. It can be assembled in the cytoplasm in the absence of the native binding protein (cytochrome *b*), and it can be assembled in truncated fragments of the Ip polypeptide which contain clusters S-1 and S-2. Based on the inferred amino acid sequence from the DNA sequence there exist three conserved clusters of cysteinyl residues which are the likely binding sites for the iron-sulfur clusters. Indirect evidence indicates that the first two of these conserved clusters, from the N terminal end, are the binding sites for iron-sulfur clusters S-1 and S-2[12].

PLANNED ACTIVITIES FOR FY 1988

Cyanobacteria and Halobacteria

In the coming year, a new NMR facility in the Life Sciences Annex will be dedicated to biological research. We forsee this as a powerful tool in our research program for the non-invasive analysis of bioenergetics and structural composition in whole cell systems. In addition, the development of new fluorescent techniques to measure intracellular pH in cyanobacteria and halobacteria will augment our non-invasive magnetic resonance investigation.

Cyanobacteria

Cytoplasmic and thylakoid membranes will be separated by established procedures, and the primary adaptive response to stress, in terms of structure and functional changes will be analyzed. Functional studies, such as ion flux, electron transport and enzyme

function, will be determined by EPR (low temperature and spin probe methods). Structural information will be derived using spin-spin interactions of membrane bound ESR probes, surface charge densities using Mn binding characteristics and by fatty acid and lipid analysis.

Succinate Dehydrogenase

Experiments will focus on succinate-quinone reductase from bacteria and mitochondria. Mechanisms and sequence of assembly of membrane metallo-enzymes are poorly understood. By using enzyme which is defective genetically, further definition of the sequence of the assembly of this enzyme will be described by measurement of an iron sulfur cluster in an enzyme fragment. Secondly, genetically defective enzyme, which is inactive enzymatically, but has defined prosthetic groups attached, will be hybridized with selected native and mutated enzyme fragments. Expression of enzymatic activity will be used to assess the essential enzyme constituents required for assembly of an intact enzyme.

The enzyme complex consists of six distinct electron/hydrogen carriers, and the pathways of electron flow will be studied using photo-reduction, laser flash photolysis and EPR to define electron flow sequences, using native and mutated enzyme. Succinate-quinone reductase from the bacterial membrane will be purified as the first step toward determining the crystal structure of this enzyme complex.

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Development and Application of New Assays of Oxidative Damage*

R.J. Mehlhorn, K. Moore, B. Stone, J. Fuchs and L. Packer

This project is concerned with the development of sensitive and specific assays for oxidative damage in biological systems. These assays are being used to measure free radicals and other oxidants that arise during normal mammalian metabolism and under pathological conditions.

ACCOMPLISHMENTS DURING FY 1987

Electron Spin Resonance (ESR) Traps for Free Radicals

Free radicals are highly reactive molecules that are produced when molecular bonds are broken. They are responsible for the lethal effects of ionizing radiation. More recently, free radicals associated with normal or abnormal metabolism have been implicated in disease and, possibly, aging, and this has led to great interest in understanding and ameliorating the effects of these adventitious free radicals.[1] Because of their high chemical reactivity, free radicals do not accumulate sufficiently to be observable. This problem has recently been solved by the introduction of "spin traps," molecules that stabilize free radicals so that they can be observed and identified.[2] In collaboration with K. Hideg of Pecs, Hungary, we have synthesized a free radical trap that offers considerably greater stability than previously available spin traps. The new compound is shown in a reaction with the very destructive hydroxyl radical as shown in Figure 1.

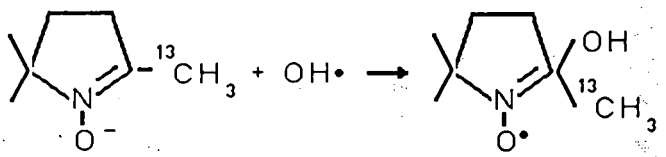

Figure 1. Reaction of the carbon-13 spin trap with the hydroxyl radical. (XBL 881-146)

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In this reaction the hydroxyl radical adds to the unsaturated carbon position in the ring, forming a nitroxide free radical, which is considerably more stable than the initial hydroxyl radical and can be observed in an ESR instrument. The introduction of a carbon-13 methyl group into the spin trap ensures that a free radical adduct will not be susceptible to further oxidation, resulting in the enhanced stability of this trap compared to previously available reagents. Moreover, the nuclear spin on the carbon-13 interacts with the unpaired electron in the free radical to yield distinctive spectra for different radical adducts that serve to identify the chemical structures of free radicals that have been trapped. This is illustrated in Figure 2, where reaction products of the new spin trap with three different, biologically important, free radical species are shown.

Detection of Free Radicals and Transition Metal Ions with Hydroxylamines Derived from Nitroxides

Nitroxide "stable" free radicals, although highly persistent in biological environments, are susceptible to reduction by one-electron donors, resulting in hydroxylamines. These hydroxylamines are

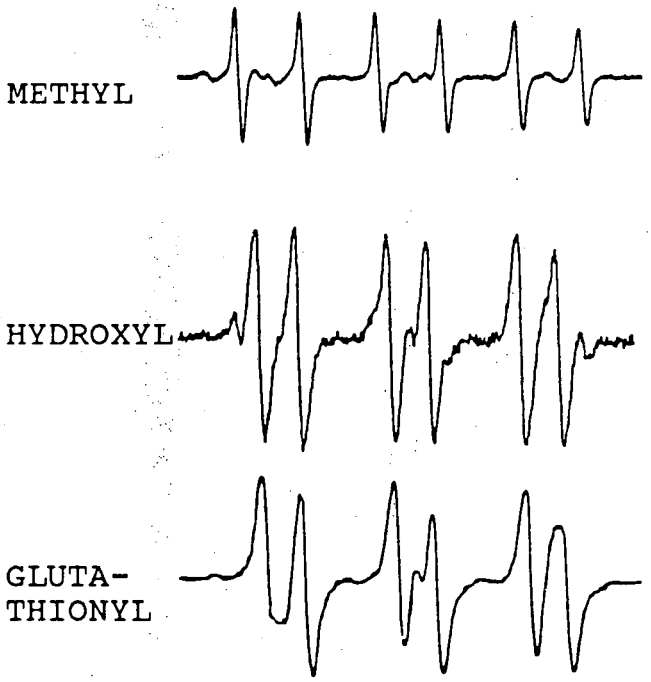

Figure 2. ESR spectra of three free radical adducts with the carbon-13 spin trap, demonstrating that biologically important oxidants can be identified with this tool. (XBL 881-145)

readily re-oxidized by a variety of free radicals and transition metal ions. We have shown that both the reduction and oxidation can be used to study free radical processes. Recently, we showed that comparative studies of reduction rates of nitroxides of different structures can be used to discriminate between major reducing agents in biological tissues.[3] We observed that ascorbic acid, which has generally been considered to be the most important reductant for nitroxides in animal tissues is a potent reductant for the piperidine nitroxide Tempol, but has little effect on pyrroline nitroxides. On the other hand, reduced flavin mononucleotide (FMN), which is a more powerful reducing agent reduces both piperidine and pyrroline nitroxides at comparable rates. From this reduction study we concluded that an analysis of reduction rates of different nitroxides can be used to analyze biological tissues for their content of ascorbate and other reductants.

Hydroxylamines derived from nitroxides by chemical reduction have proven useful for the detection of one-electron oxidants, including free radicals. In particular, we have observed that the hydroxylamine derived by a one-electron reduction from 2,2,6,6-tetramethyl-piperi-dinoxyl-4-ol (Tempol), designated as TOLH, is oxidized by phenoxyl radicals. We have exploited this fact to develop TOLH as a tool to detect oxyl radicals. In addition, we have found that TOLH oxidation, in the presence of the enzyme horseradish peroxidase and micromolar concentrations of phenol, can be used for the quantitative determination of hydrogen peroxide in tissue homogenates and cell fractions.

We have also observed that the oxidation of TOLH is mediated by traces of copper and iron ions, an effect that is strongly modulated by chelating agents. This observation has led us to develop an assay for the presence of free transition metal ions in biological systems. The assay consists of measuring the rate of TOLH oxidation in the presence and absence of membrane-permeable chelating agents that sequester the ions. The possibility that transition metal ions might be free in cells has been of great interest because of their potential as sources of free radicals in the presence of hydrogen peroxide. Among promising new research opportunities, this tool will enable us to determine whether there are pathological conditions or environmental stresses that cause such ions to be released in cells and whether there are drugs that can prevent their harmful effects.

Free Radical Traps that Produce Volatile Products

While free radical studies *in vitro*, such as those that can be obtained with spin trapping, are very useful for inferring reaction mechanisms, it is generally acknowledged that the *in vivo* implications of such studies, particularly for higher animals, are clouded by the complexity and diversity of possible responses of multicellular organisms to oxidative stress. Therefore, the development of oxidative damage indicators that report on the net effect of some stress on higher animals has been of considerable interest. Among the most encouraging recent developments are highly sophisticated analytical tools for detecting oxidation products in urine and in breath.[4] We have been interested in the potential of breath analysis, both as a research tool and as clinical diagnostic aid. A review of the current state-of-the-art has led us to identify a promising breath analysis research tool that offers high sensitivity and specificity. In collaboration with H. Rapoport of LBL, we are developing a novel radiolabeled free radical trap, tritiated 4-keto thiometyl butyric acid (KTBA), which will fragment into several products after reaction, liberating a radiolabeled gas that can be collected in the expired breath of an animal.

Free Radicals and Antioxidants in Skin

We investigated the free radical-reducing activity in skin, using nitroxide radicals as model compounds for endogenous radicals. The skin was derived from hairless mice. Nitroxide reduction rates vary considerably depending on the structure of the nitroxide. Five-membered ring pyrroline nitroxides exhibit consistently better stability than six-membered ring piperidine nitroxides. The substantially higher reduction rate observed for six-membered rings in mouse skin suggested a major role for ascorbic acid as a free radical reducing agent. This inference was confirmed by treating skin homogenates with ascorbate oxidase, which greatly inhibited reduction of the nitroxides. However, an appreciable reduction rate was observed for even the most stable five-membered rings, indicating that non-ascorbate reduction is an important alternative pathway for reducing nitroxides in skin. Among these non-ascorbate reduction pathways, thiols appear to play a major role, since treatment of skin homogenates with the thiol reagent N-ethyl maleimide substantially inhibited reduction.

PLANNED ACTIVITIES FOR FY 1988

The new traps being synthesized will be tested in both model systems, including transition metal catalyzed hydroxyl radical generators, peroxiding lipids in model membranes, cellular and subcellular systems, e.g., erythrocytes and mitochondria, and animals (rats). We will establish the sensitivities and specificities of the assays and seek to quantitate "background levels" of free radicals that occur in the absence of stress. This will set the stage for analyzing oxidative damage associated with stress, including the effects of gaseous substances like ozone and radon, water-borne hazards like heavy metals and organic pollutants, and free radical sources of clinical interest, e.g., ionizing radiation, hyperbaric oxygen and quinone anticancer drugs. These studies will extend into future years.

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Impacts of Large Extraterrestrial Bodies and Mass Extinctions*

F. Asaro, H.V. Michel, W. Alvarez and L.W. Alvarez

Two enormous Ir anomalies are found in Archaean spherule-enriched layers in South Africa. Chemical measurements suggest an impact source is currently the most viable explanation.

New measurements have shown there are distinct small Ir peaks directly above the huge K-T Ir spike which disappear when ratios to clay abundances are taken. The resulting curve is continuous (as well as nearly exponential), and the smooth nature precludes episodic volcanism as a cause.

In studies of the limestone sediments near Gubbio, Italy over a 5 million-year span, only the region within about 1-1/2 meters of the K-T boundary shows any Ir anomalies above the background of ~ 13 ppt.

ACCOMPLISHMENTS DURING FY 1987

In collaboration with Donald R. Lowe and Gary R. Byerly from Louisiana State University (LSU), we have made a detailed chemical study on 104 Early Archaean (~ 3.5 billion years old) rock samples from South Africa and Western Australia. Two layers of spherule-bearing rocks in South Africa were found to have enormous enrichments of Ir. The lower layer, near the base of the Fig Tree (geological) Group of the Barberton Greenstone Belt, had up to 76 parts-per-billion of iridium (Ir) per gram of rock (ppt) and the upper layer, which varied from 50 to 200 meters higher than the lower, had up to 162 ppb. The Ir content varied considerably in different sections and was inversely correlated with reworking by current activity.

Studies of ultramafic rocks in the Greenstone Belt showed much lower levels of Ir than the maxima found in the spherule beds and argue against a volcanic origin. The measurement of 28 other elements by high precision, neutron activation analysis techniques at LBL and other elements by x-ray fluorescence at LSU suggest the impact of a large asteroid or comet is the most viable explanation for the spherules. More definitive measurements are needed, particularly of the abundances of other platinum group elements, to critically test this hypothesis.

A spherule bed found in the Warrawoona Group of the Eastern Pilbara Block in Western Australia contained up to 4.5 ppb Ir. These spherules may also have been caused by impact but the evidence is not as strong as for the South Africa beds.

A geochemical study has been made of nearly 60 meters of limestone covering over 5 million years of deposition near the Cretaceous-Tertiary (K-T) boundary in the Bottaccione Gorge near Gubbio, Italy. Except in 2.6 meters of rock directly adjacent to the huge K-T Ir spike, no Ir anomalies were observed, and the average Ir background was 12.6 x 10^{-12} gram of Ir per gram of rock (ppt).

Close to the K-T spike of ~ 3000 ppt Ir, there are 7 peaks above and 5 peaks below ranging from 20 to 80 ppt Ir above background. Above the boundary, the Tertiary peaks disappear if ratios are taken with respect to abundance of elements in clay, e.g., Fe, Si, and Al. The curve, which corresponds to carbonate-free measurements, shows essentially a continuous exponential dropoff from a few cm to 1.4 meters above the boundary. The continuous nature of the curve suggests that the source of the Ir was not episodic, i.e., was not due to volcanism. Washing of the continents following the impact of a large asteroid or comet would produce an exponential decrease in Ir abundance in the sediments as a function of time if the Ir available for erosion on the continents decreased by a constant fraction for each unit of time, i.e., the exponential decay of radioactive isotopes.

If the explanation for the Tertiary effects is correct, we would not expect to see the same mechanism in the Cretaceous rock under the K-T spike because Ir obviously could not be washed off the continents before the K-T impact. When ratios are taken to the clay elements for the Cretaceous Ir peaks, they do not disappear as in the Tertiary and, in addition, appear broader and periodic. The Ir tail under the peak is also much smaller than in the Tertiary. We are currently investigating whether diffusion of the iridium downward accompanied by band-

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ing, e.g. Liesegang banding of iron in sediments, might explain the Cretaceous peaks.

The peaking of Ir and clay elements in the Tertiary rock (in contrast to the smooth nature of their ratios) may be due to rhythmic dissolution of $CaCO_3$ triggered by the presence of the soft K-T boundary clay between the hard limestone formations. The boundary clay itself is in large part detrital with a component of impact debris (Ir, spherules, and shocked quartz), and we are investigating whether it may be due to pressure dissolution of ~ 10 cm of limestone triggered by the presence of impact debris. The presence of clay is known to encourage pressure dissolution of limestone.

PLANNED ACTIVITIES FOR FY 1988

We will collect, prepare and study about 1100 samples from deep sea cores ODP (Ocean Drilling Project) 689B and 690C taken from the Weddell Sea near Antarctica. The presumed Cretaceous-Tertiary (K-T) boundary regions in these cores have volcanic ash debris, and we want to determine if volcanism accompanied the K-T impact. We will also look for the Late Eocene (conventionally ~ 39.5 million years old) Ir anomaly that we have previously seen only as far south as 36° south latitude. ODP 689B was taken from ~ 64° south latitude. We will look for a Middle Miocene (~ 11.7 million years old) Ir anomaly in the same core which we have so far seen in only one site about 10,000 kilometers away in the Tasman sea.

We will also study a suite of ~ 600 samples (from near and above the 225 million years old Permian-Triassic boundary) collected in China for a Chinese-U.S. cooperative project that we helped organize.

Source Determination of Archaeological Obsidian in Mesoamerica*

F.H. Stross, H.V. Michel, F. Asaro

The neutron activation and the x-ray fluorescence equipment continue to be used for studying trade patterns and their historical implications in Pre-Columbian Central America. Obsidian artifacts, among trade items least affected by time and climate, have been the main objects of our studies in this connection.

*This research was supported by the Council on Research and Creative Work of the University of Colorado, the Quirigua Project of the University of Pennsylvania Museum, The National Science Foundation, the Trent University Research Committee, The National Geographic Society, The University of Texas Institute of Texan Culture, The Department of Sociology and Anthropology at the Southwestern Texas State University, The Social Sciences and Humanities Research Council of Canada, The University of California, Santa Barbara, The Centro Regional de Yucatan of the Institute Nacional de Antropologia e Historia of Mexico, Mr. & Mrs. Fifield of Milwaukee, Wisconsin, The President's Council of the University of Florida, The Instituto de Antropologia e Historia of Guatemala, The Peabody Museum (Harvard), The Wheelerbrator-Frye Foundation, Mr. Thomas Begel, The University of North Dakota Anthropology General Research Fund and Faculty Research Committees, and the Patrimonio Cultural of El Salvador.

ACCOMPLISHMENTS DURING FY 1987

Careful analytical studies can locate the sources of the raw materials of obsidian artifacts excavated in archaeological sites having access to the volcanic regions in which this natural glass is found. Trade distribution patterns, and their changes with time, can thus be determined; they provide valuable information relating to the history of the regions studied.

Raw materials of obisidian artifacts excavated in Belize, Nicaragua, Honduras, and Costa Rica were found to derive largely from the Guatemalan Highlands, but they included two distinctive groups of unknown origin. The sources of the latter have now been identified and found to be located at La Esperanza and Guinope, both not far from Tegucigalpa. It is remarkable, though unexplained, that although obsidian artifacts from these sources have been found in the regions mentioned above, no artifacts matching the Honduras sources have so far been found in archaeological sites located in the rich Maya centers of Guatemala and Mexico. It is not known if the quality of the obsidian, transportation problem, power-derived monopolies, or other reasons resulted in the uneven distribution of the Honduran obsidian.

While most of the interest in the Maya culture in the past has focused on such rich and spectacular ceremonial sites as Tikal, Palenque, Kaminaljuyu, Yaxchilan, Copan, and their satellites, more recent

projects have dealt increasingly with habitation areas and ports of trade. The latter types of sites may yield less dramatic remains, but more significant information in terms of the daily life of the peoples involved.

The areas studied include inland and off-shore Belize, the Northern Peten, Honduras, Nicaragua and a small island north of Yucatan. The trade distributions shifting with time presumably reflect changes in power structures and other important factors in the history of the Maya. The sites located in the present Belize and the nearby Peten (Guatemala) areas showed distribution patterns foreshadowed in earlier studies: Predominance of the Rio Pixcaya source in the Preclassic periods (before 250 AD) shifted to the El Chayal flow during the Classic (ca 250-900), then to the Ixtepeque source in the terminal Classic and Postclassic (ca 750-1200). These sources are located in the Guatemalan Highlands; very few artifacts derived from Mexico.

Isla Cerritos, just off the northern coast of Yucatan, appears to have been the main port-of-trade for the great site of Chichen Itza in Yucatan. In accord with what is known of the history of this latter site, nearly all of the artifacts found could be dated to relatively late periods, i.e. to terminal Classic and Postclassic. In the suite of artifacts excavated in Isla Cerritos, less than 20% derived from the Guatemalan Highlands, while essentially all of the remaining specimens derived from sources in present-day Mexico. This reflects the presumed incursion of the sites by the Toltecs, who established themselves in Chichen Itza during the period indicated, and left their dramatic mark on that site.

The directors and co-directors of the excavating projects included P. Sheets, F. Lange, K. Hirth, H. McKillop, A. Andrews, W. R. Fowler, P. F. Healy, T. R. Hester, and T. H. Guderjan.

PLANNED ACTIVITIES FOR FY 1988

Interest in Mayan field studies has been shifting toward the southeastern regions of their domain. Pre-Columbian sites in Belize, Honduras, Nicaragua, and Costa Rica recently excavated are furnishing new material on segments of the Maya culture that had not been available so far, and our collaborative research is expected to continue along these lines.

Measurement of Femtogram Quantities of Trace Elements Using an X-ray*

R.D. Giauque, A.C. Thompson, J.H. Underwood, Y. Wu, K.W. Jones [†], and M.L. Rivers [‡]

The development of intense synchrotron radiation beams has led to significant interest in their application for the measurement of trace element concentrations of very small specimens by x-ray fluorescence. Sparks[1] reported the use of an x-ray fluorescence microprobe using synchrotron radiation for the analysis of monazite giant halo inclusions in biotite in the search for superheavy primordial elements. A curved mosaic graphite crystal was employed to both focus and monochromatize the synchrotron radiation beam. Photons of energy 37 keV with a full width at half maximum (FWHM) of 0.4 keV were used. A flux of 15 x 10^{10} photons /(s mm^2) was realized. The actual beam spot size was 0.64 mm^2.

Since 1981 a number of papers have been published regarding the use of x-ray microprobes[2-5]. In most cases, the synchrotron white radiation beam has been collimated using vertical and horizontal slits or doubly curved crystals have been used to focus the radiation. Typical useable beam spot sizes attained are on the order of 700 - 2500 μm^2. More recently Iida and Gohshi[6] have demonstrated the use of a reflection/transmission mirror combination to focus and monochromatize synchrotron radiation. Using an irradiation area of 3500 μm^2, a MDL of 0.03 pg was ascertained for Zn adsorbed on chelate.

*This work was supported by the Office of Energy Research, Office of Health and Environmental Research of the U.S. Department of Energy under contract DE-AC03-76SF00098. The experiment was carried out at the NSLS X-26C beam line which is supported by the Office of Basic Energy Sciences, Chemical Sciences Division, Processes and Techniques Branch of the U.S. Department of Energy Contract No. DE-AC02-76CH00016; the National Institutes of Health as a Biotechnology Research Resource, Grant No. P41RR01838; and the National Science Foundation, Grant No. EAR-8618346.

[†]Brookhaven National Laboratory, Upton, NY 11973

[‡]University of Chicago, Chicago, IL 60637

ACCOMPLISHMENTS DURING FY 1987

The application of an x-ray microprobe that permits very high analytical sensitivities to be realized with improved spatial resolution is described. The instrument permits the spatial distribution measurement of femtogram quantities of trace elements using count intervals of 60 s or less per 10 μm x 10 μm pixel. Calibration of the microprobe was accomplished using National Bureau of Standards thin glass film Standard Reference Materials. A variety of specimens have been scanned to demonstrate the applications that are possible with this microprobe.

The experiments were carried out at the Brookhaven National Synchrotron Light Source (NSLS). White radiation was used as the primary source for the measurements undertaken. The microprobe that was employed to serve as a wide bandpass monochromator and focus the x-ray beam is illustrated in Figure 1. The principal components of the instrument are a pair of concave spherical mirrors coated with tungsten-carbon multilayers. The mirrors are arranged in the Kirkpatrick-Baez geometry. The focusing elements were "super-polished" quartz mirrors with a 6 m concave spherical radius of curvature. Using a dual source sputtering system, each mirror was coated with tungsten-carbon multilayer pairs. The mirror nearest the synchrotron radiation source was coated with 200 multilayer pairs. The second mirror was coated with 100 multilayer pairs. The 2d spacings of the tungsten-carbon multilayer coated mirrors were 58 Å and 87 Å, respectively. The above thicknesses for the multilayer pairs were designed to allow 10 keV radiation to be efficiently reflected when the mirrors were properly aligned. The bandpass of the mirrors was 1 keV and the focused beam spot was less than 10 x 10 μm. A more detailed description of the x-ray microprobe has been reported[7].

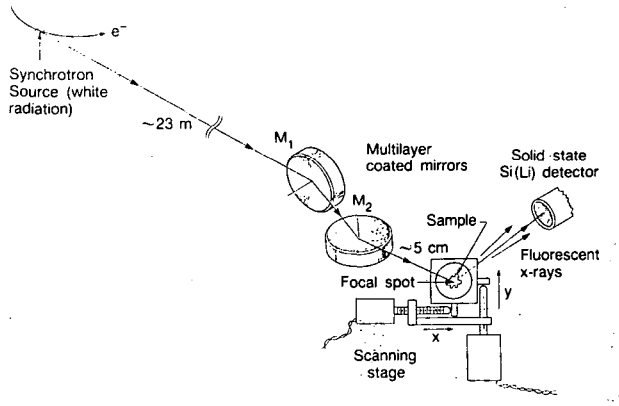

Figure 1. Schematic of the x-ray microprobe. The pair of concave spherical mirrors are coated with tungsten-carbon multilayers. (XBL 876-3046)

Specimens to be scanned were mounted in holders that positioned the specimen at an angle of 45 degrees relative to the incident focused synchrotron radiation beam. A scanning stage allowed the specimen to be translated with respect to the beam spot with step sizes as small as 1 μ in both horizontal and vertical directions. A 5 mm thick, 30 mm^2 Si(Li) detector was aligned so that it was at the beam height and at 90 degrees to the path of the incident radiation. An effective solid angle of $\Omega/4\pi$ = 1.8 x 10^{-3} was viewed by the detector. The synchrotron was operated at 2.5 GeV with a maximum stored electron current of 150 mA. A maximum incident flux of 3 x 10^9/s was measured for 10 keV photons in the focused beam spot.

An optical microscope, coupled to a television camera, was used to aid in the positioning of the specimen. Two National Bureau of Standards (NBS) thin glass film Standard Reference Materials, SRM 1832 and 1833 were use to calibrate the system. For our experiments, the reference materials were used to calibrate for the measurement of elements K (Z = 19) through Zn (Z = 30).

Specimens were mounted between two pieces of 6.3 μm polypropylene film that was stretched by a lucite snap ring in a lucite holder. Measurements were made for a single strand of blue green algae cells, freeze-dried thin sections of melanoma tissue from a rat, lung tissue, individual blood red cells, and minute liquid inclusions in laboratory generated quartz specimens.

To establish the minimum detectable limits of the microprobe, x-ray spectral backgrounds were acquired for scattering from air plus two pieces of 6.3 μm polypropylene film. Based on the integrals over the peak locations, Table 1 lists the theoretical (3σ) detection limits ascertained for 60 s live time

Table 1. Minimum Detectable Limits at NSLS

Element	fg/(10 x 10 μm)
K	70
Ca	20
Ti	8
Mn	3
Fe	3
Ni	2
Cu	3
Zn	3

count intervals at a beam current of 150 mA. These very high sensitivity detection limits achieved are applicable for the measurement of trace elements in a thin specimen such as a few biological cells. For biological tissue thin sections of mass thickness 1 mg/cm^2, the minimum detectable limits for these same elements vary between 1 and 40 ppm. For these latter specimens, the intensity of the scattered excitation radiation may be used as a measure of the specimen mass in the beam spot[8] and therefore provide information necessary to determine the concentrations of the elements measured.

As an illustration of the sensitivity of this instrument, a single strand of blue green algae cells was scanned lengthwise in 10 μm steps using count intervals of 30 s per pixel. The size of the individual cells was 3 to 4 μm. Thus, typically three to four cells were in the beam path for each pixel. Figure 2 is a spectrum obtained for one pixel. The elemental quantities listed are in pg. The spectrum clearly shows Mn and Ni at 30 and 20 fg/100 μm^2 level, respectively. The results of an 11 pixel scan along the center of the cell strand are summarized in Figure 3. The initial results obtained clearly demonstrate the high sensitivity and spatial imaging capability of the x-ray microprobe to measure femtogram quantities of specific elements within a 10 x 10 μm beam spot. Additionally, trace element determinations at the ppm concentration level are feasible for thin sections of biological tissues.

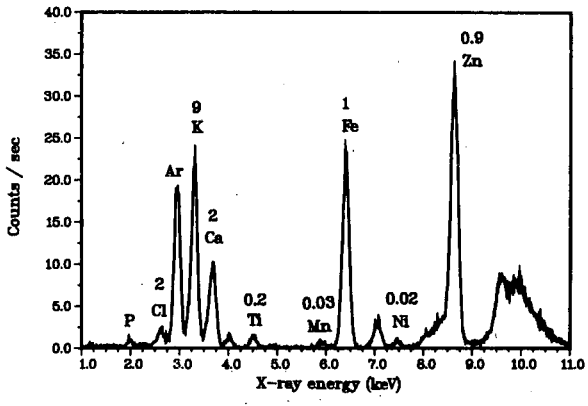

Figure 2. Spectrum obtained in 30 s for a 10 μm x 10 μm pixel of a single strand of blue green algae cells. The element quantities listed above the spectral x-ray lines are in pg. (XBL 876-3045)

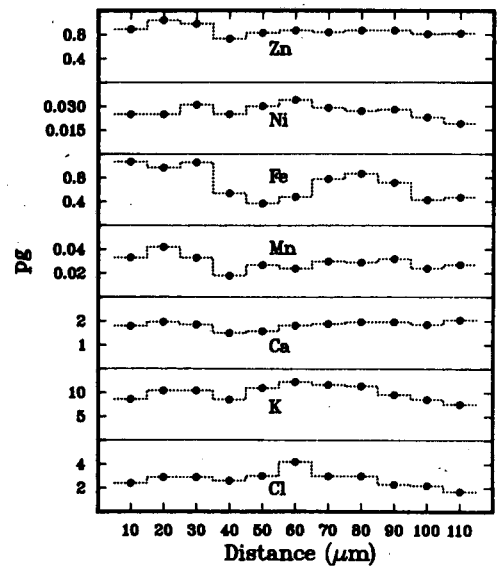

Figure 3. Summary of results ascertained from a scan lengthwise, in 10 μm steps, along the center of a strand of blue green algae cells. (XBL 876-3048)

PLANNED ACTIVITIES FOR FY 1988

Plans are currently being made to fabricate improved mirrors which would give a focused beam spot of a few square microns without any significant loss in x-ray flux. With these mirrors, concentrations of many trace metals in individual biological cells could be ascertained. Such an instrument would be a powerful analytical tool for a variety of research programs. Furthermore, since the specimens are not under vacuum, the x-ray microprobe can accommodate specimens that cannot be studied with an electron microprobe.

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ENERGY ANALYSIS PROGRAM

INTRODUCTION

FY 1987 was an eventful year, both for energy policy and for LBL's Energy Analysis Program (EAP). One of the most discussed issues in U.S. energy policy has been the structure of the electric utility industry. The extraordinary boom in offers to construct cogenerators and other qualifying facilities under the Public Utilities Regulatory Policies Act (PURPA) during the past several years, combined with an apparent aversion by utilities to invest in power plants, has led to serious discussion about, and analysis of, utility deregulation, especially supply. This topic is of great importance both in terms of influencing future electricity supply and use and in their effects on U.S. capital markets, with the electricity industry traditionally the most capital intensive industry in the U.S. EAP has played a significant role in analyzing utility issues during the year. A major report for the Policy Office of the U.S. Department of Energy (DOE) analyzed bidding procedures (auctions) as a means of increasing the economic efficiency of PURPA purchases (see article by Rothkopf and Kahn). Such an approach is not only important for improving PURPA; it could also be an important element in a broader strategy to deregulate, or partially deregulate, utilities. The Least Cost Utility Planning Project (LCUP), supported by the Office of Buildings and Community Systems of DOE has also contributed important insights into issues shaping the electric utility industry. LCUP has delved deeply into demand-side options and programs of utilities (article by Krause) and has analyzed how such programs fit in an integrated planning framework (article by Kahn, *et al.*).

During the past year, the U.S. Congress took the first action since the 1970's in initiating a major energy conservation policy. This was the passage of the National Appliance Energy Conservation Act (NAECA). NAECA set minimum mandatory standards for major energy-using residential appliances, including furnaces and air conditioners. The Act resolved and rendered moot a Federal Appellate Court decision requiring DOE to set standards. EAP leads the overall federal appliance standards research program. EAP researchers analyzed the impacts of NAECA. The article by Ruderman, *et al.*, estimates 0.7 to 1 quad per year energy savings after the turn of the century and demonstrates substantial consumer benefits of NAECA. The Congressional Act also requires DOE to decide on standards for several products. The EAP team's analysis will constitute the major technical input to these decisions, the most controversial of which will concern standard levels for refrigerators.

A third energy policy area of intense national interest derives from the continuing low price of liquid fuels—up from 1986 but still much lower than previous years—and the energy security issues arising from anticipated future tight oil markets and heavy reliance on Middle Eastern OPEC oil. This area of concern has been dramatized by a major DOE report entitled *Energy Security: A Report to the President of the United States.* EAP research contributed directly to this report in highlighting the rapid increase in oil use in developing countries. The data collected and analyzed by the International Energy Studies (IES) Group suggested that future oil demand in developing countries is likely to be higher than commonly recognized. A major outcome of the high-level DOE review of energy vulnerability issues has been a decision to pursue a major study of alternatives to oil for transportation fuels. This project, a major new initiative of the DOE Policy Office, will be managed by EAP staff.

In addition to work directly related to key current energy policy issues, EAP continued research in a wide variety of areas, deepening our understanding of topics that have been investigated over many years. The Building Energy Analysis (BEA) Group, under Ron Ritschard, continued its analysis of energy use in public housing (an area much in need of improvements in energy efficiency), improved and extended its data base and simplified tools (including home energy rating systems) for assessing residential energy use, and gained new knowledge through several special studies (on residential foundation design, vegetative cover as a conservation strategy, and air-to-air heat exchangers). During the coming year, the group is expected to apply its capabilities to multifamily and commercial buildings.

The Energy Conservation Policy (ECP) Group, under Mark Levine, continued to focus its emphasis

in three major areas: appliance standards; energy conservation research and policies for buildings in Southeast Asia; and economic studies of electric utility demand-side programs. In the first two areas, substantial progress was made in getting the research incorporated into ongoing policy processes. The utility research is evolving in two different directions: (1) broader studies of integrated utility planning issues and (2) more detailed studies of end use data relevant to residential and commercial load shapes. The latter topic is an important input into utility planning.

The International Energy Studies (IES) Group (co-led by Jayant Sathaye and Andrea Ketoff until Lee Schipper's return late in FY 1987) split its efforts between research on energy in LDC and OECD nations. The Group expanded its work to include a variety of supply issues in addition to its traditional (and continuing) strong emphasis on factors underlying energy demand. An important new initiative of the IES Group was the creation of an International Energy Roundtable. This Roundtable, involving meetings and discussions among high-level energy analysts from developing and developed countries, dealt with key international issues during the year.

The Buildings Energy Data (BED) Group, under Jeff Harris, continued its research efforts to better characterize the energy use of buildings from measured data. In addition to improving the data bases (particularly for multifamily and new residential buildings), BED also studied several emerging energy conservation technologies (thermal energy storage, variable-speed motor drives, and energy management systems), analyzed in depth the problem of urban "heat islands", and evaluated end-use data and utility conservation programs in the Least Cost Utility Project. An important new undertaking is the application of statistical methods to BED's building-specific energy data bases to begin to draw inferences about the potential for increasing energy efficiency of the U.S. building stock.

The Resource Market Mechanisms area, under Mike Rothkopf, was actively involved in a number of key national policy issues. The major contribution, discussed earlier, was the innovative research on different bidding procedures as a means of improving the PURPA process.

A major new area for the Program was initiated during FY 1987: environmental policy analysis. Two experienced researchers in this field, Walter Westman and Paolo Ricci, have been recruited and will begin work in early FY 1988. The key areas of research emphasis have been defined to include risk assessment of environmental pollutants, effects of changes in global climate, and studies of ecological effects of environmental stressors. A dialogue has begun, both with policy and research personnel in the federal government and with researchers within the UC system, to lay the groundwork for this new activity which will contribute to research and analysis of emerging national and international environmental policy issues.

BUILDING ENERGY ANALYSIS

Overview

The Building Energy Analysis Group (BEA) conducts research and analyses on all important issues relating to the use and conservation of energy in residential buildings. The work stresses *whole buildings* rather than individual components viewed separately, in an effort to improve understanding of the tradeoffs among different approaches to achieve increased efficiency of building energy use. The research is intended for two types of use: (1) *to further knowledge* of all aspects of energy use in residential buildings and (2) *to provide research results* in a simplified format to assist builders and building operators to reduce energy use in residences. The work of the Group focuses on four areas:

- Simplified energy analysis methods,
- Energy-efficient and cost-effective cooling strategies,
- Residential building type analysis (single and multifamily), and
- Public and low-income housing.

A major accomplishment of the Group is the development of a simplified computer energy analysis tool (PEAR), which serves as the calculation procedure the Department of Energy's voluntary guidelines for new residences and the source of energy requirements for the revisions to the ASHRAE 90.2 standard. An article by Huang, Bull and Ritschard describes revisions to the residential data base used to support PEAR that were developed for Pacific Northwest Laboratories in conjunction with ASHRAE, and with support from DOE. Another part of the revised data base is described in an article by Huang and Bull and these revisions include simulating below-grade heat flows using a method developed by the University of Minnesota in conjunction with the DOE-2.1C program to determine the conservation potential of different foundation measures.

Another important research topic in support of developing simplified energy analysis tools considered existing residences and the use of home energy and labeling systems. An article by Ritschard, Vine, Barnes *et al.*, reports on the evaluation of a demonstration program sponsored by the California Energy Commission on rating and labeling existing homes in two California cities: Pasadena and Roseville. In a second article in this area, Vine, Barnes and Ritschard provide a broader evaluation of 34 home energy rating systems in 28 states.

In addition to gaining an better understanding of the energy performance of single-family residences, the BEA Group has been conducting research on the topic of existing multifamily buildings, particularly in the public housing sector. Two studies are presented for FY 1987. First, Ritschard, Greely, Goldman, Mills, and Vine provide an overview of the federally-assisted housing program that covered three activities this year in support of the overall goal of improving energy efficiency of public housing. Finally, Greely, Mills, Goldman, and Ritschard present results of a study of energy use at 91 selected public housing projects across the U.S. using both utility billing data and oil consumption data.

California Home Energy Rating and Labeling Demonstration Program: What Did We Learn?*

R. Ritschard, E. Vine, B.K. Barnes, C. Hsui, and I. Reyes

Homes built prior to California's energy efficiency standards for new residential buildings (1978) will still comprise a majority of California's housing stock by the year 2000. If homeowners were to retrofit these existing homes by increasing attic and wall insulation, improving water heating practices, and installing storm windows, setback thermostats, and other retrofit measures, the state's total residential natural gas and electricity consumption could be reduced by as much as 29%.[1] More importantly, homeowners could collectively save as much as $18 billion in the next ten years.

Many barriers exist to this type of home improvement. For example, lenders, while they may understand that greater energy efficiency leads to lower utility bills, lack a standardized method of accurately including energy efficiency in the "comparable value" of the home. One strategy for overcoming this barrier is a method for rating and labeling existing homes on the basis of their energy efficiency. By using a simple numerical scale, different sizes and types of homes can easily be compared and advertised.

To explore these benefits, the California Energy Commission (CEC) sponsored a *demonstration* program during 1985 and 1986 on rating and labeling existing homes in two California cities: Pasadena and Roseville. The goal of the project was to evaluate various delivery mechanisms that might be used in conjunction with a statewide home energy rating and labeling program. Another goal was to develop a single rating tool which could, with reasonable accuracy, rank the energy efficiency of any home within the state.

ACCOMPLISHMENTS DURING FY 1987

A major element of the CEC's Demonstration Program was the Rating Tool developed previously by LBL.[2] The primary intent of the tool was to provide accurate estimates of each building component's contribution to the overall energy use of the house in a simplified manner. The tool used a slide rule format to provide a simple and easy-to-understand way for translating the house characteristics into an energy rating. The final calculated values from the slide rule were compared to a rating scale, which was a normalized scale from 1 (least energy efficient) to 6 (most energy efficient). The scale was set using the estimated energy budget for a house that met California's 1978 new building standard as a "3", and a current Title 24 house as a "5". The ratings were scaled linearly from these two benchmarks so that the estimated incremental savings are the same between any two ratings.

The Cities of Pasadena and Roseville were selected by the CEC to test two different delivery mechanisms. Pasadena, as the model for a *government-focused* delivery mechanism, used city building officials to certify a home's rating and provide labels. Roseville was selected to implement a *utility-focused* program in which the city, as an electric utility, offered a home rating and labeling service. In both Pasadena and Roseville, the ratings were provided by trained energy auditors. Pasadena was to have had a second program using building inspectors, but there was a potential conflict of interest: building inspectors are obliged to report building code violations, and this obligation may compromise the program by threatening the homeowner in reporting violations and adding certain liability problems for building officials in guaranteeing the ratings.

Both Pasadena and Roseville projects involved raters whose job it was to audit houses and provide information to homeowners about improving the energy efficiency of their homes. The Pasadena project used two auditors who independently rated 25 city employee's houses during June and July 1986. In Roseville, a single auditor (RCS-trained) rated 68 houses between December 1985 and September 1986. The Roseville ratings were performed as part of the energy audit mandated by a city ordinance requiring that all houses built prior to July 1978 be audited upon resale.

LBL evaluated the rater's experience with the Rating Tool and the delivery systems used in each demonstration project by addressing three principal questions:[3]

(1) Does the Rating Tool work?
(2) Who should do the rating?
(3) How can the effectiveness of the rating process be improved?

In addition to reviewing evaluation reports submitted by the two cities, we collected data on the

*This work was supported by the Conservation Division of the California Energy Commission under Contract No. 400-84-002 through the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.

demonstration programs by interviewing homeowners, real estate agents, raters, and program managers. The interviews were conducted by telephone, and a structured questionnaire containing open-ended and closed-ended questions was used. We found that the testing of the Rating Tool itself became the focus of the demonstration programs; the development of a comprehensive delivery mechanism received little attention.

The raters in both cities were generally very favorable to the Rating Tool; they thought it was easy to understand and simple to use, comprehensive, provided a rating in a reasonably short time period, and could be a great boon to their profession. Some technical problems were encountered with the tool itself such as, accounting for window air-conditioners, and developing additional efficiency level for heat pumps.

Other problems were encountered that were more subjective in nature, but which could be treated in a consistent manner with guidelines and proper training of raters (e.g., determining infiltration levels, and estimating the area of shaded windows). After confronting these problems and arriving at tentative solutions, the raters were able to continue to use the tool and perform the rating calculations. Moreover, based on program reports by the two cities and on our interviews with raters and program coordinators, there appeared to be *no* insurmountable problems associated with the continued use of the Rating Tool in these communities.

Based on the responses of the project coordinators in Pasadena and Roseville, the experience of the raters, real estate agents, and homeowners, and pulling together conclusions from our own investigation of HERS, on a national basis, (see Annual Report article by Vine, *et al.*), we make several recommendations.

First, the CEC/LBL Home Energy Rating Tool worked but it can be improved with some technical modifications and with supporting documentation. Second, comprehensive delivery systems are necessary for successful implementation of home energy rating systems (HERS). The target of home energy rating programs (homeowners or builders) must be provided with both technical and financial assistance in order to facilitate energy-efficiency improvements as well as to motivate their investment decision. Third, raters should be trained auditors with sufficient knowledge and understanding of how homeowners make decisions on improving the energy efficiency of their home. Finally, the homeowner *must* be viewed as an active participant in the rating process rather than as a passive recipient of a HERS label. One of the key measures of the success of a home energy rating program is how much energy is saved as a result of the homeowner's implementation of energy-saving measures. It is further recommended that a rating or certification form be provided to the homeowner as a record of the rating process.

PLANNED ACTIVITIES FOR FY 1988

This research has been concluded and no further activities are planned.

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Evaluation of the Implementation of Home Energy Rating Systems*

E. Vine, B.K. Barnes, and R. Ritschard

The rating and labelling of new and existing energy-efficient homes by local, state, and federal government agencies, utility companies, and other organizations has been an activity marked by periods of intense interest and benign neglect. During the late 1970's, home energy rating systems (HERS) became important components of several energy conservation programs conducted by governmental and non-governmental organizations at national, regional, and local levels. By 1982, it seemed that the idea of a home energy rating system had become entrenched as an effective means of pursuing the goal of energy conservation. Since that time, however, a number of these systems have been abandoned, and only a few have endured. Nevertheless, a number of HERS exist, and interest in HERS has increased in selected areas of the country.

ACCOMPLISHMENTS DURING FY 1987

In January 1986, we conducted a national telephone survey of home energy rating systems to examine the different kinds of HERS and implementation systems being used and to discover the range of possible implementation problems and solutions experienced by the users of these systems. We first contacted all state energy offices in the U.S. to discover where existing HERS were operating. Major systems were followed up in each state, and we examined those operated by local governments and utility companies. We identified 28 states willing to provide examples of some form of HERS that was currently in operation.

HERS Distribution

The 28 states provided information about 34 HERS programs: 14 of these were located in the Southeast, 8 in the Midwest, 5 in the Northeast, 4 in the Pacific/Mountain region, and 3 in the Southwest. HERS seem to be concentrated mainly in those areas concerned with regulating cooling loads. Most (20) of the programs were developed at the national or regional level, 6 by states and 7 by large utility companies or energy production and distribution authorities, as compared to the local level, where 14 HERS were developed, usually, by smaller utilities. Home builders associations, in particular, have tended to play a critical role in the adoption of most successful programs, are often consulted within the development phase, and have helped implement some of the major HERS in operation.

HERS Findings

The first critical observation, based on our survey, is that it is virtually impossible to treat HERS in isolation from other energy conservation efforts. In particular, HERS' connection to auditing is often complex and inseparable. The promotion of HERS is intimately connected to the promotion of energy efficiency, and HERS are rarely offered in isolation. More frequently, a HERS is a part of an energy-efficiency package.

This diversity in HERS implementation is in part a consequence of the diversity in the target populations which range from homeowners and homebuyers (consumers) to real estate appraisers. Moreover, different expectations for, and uses of, HERS exist within these groups, and these differences affect the kinds of strategies evolved for successful implementation of HERS. Often, in the development of a particular program, the different goals and interests of participants need to be reconciled through negotiation; the alternative being the withdrawal of support by critical parties, or even the development of rival systems.

Many failed HERS started from the assumption that consumers were energy experts, and that the provision of a HERS was only viable if it met a market demand. When consumers were surveyed and found to be uninterested in energy efficiency, many energy authorities treated this information as evidence that a HERS was unwanted, unnecessary, and unviable. Accordingly, many failed HERS were typically passively operated, with little or no promotional budget, employed a tool that could not evaluate alternative paths to energy efficiency and that presented the rating in a way that had little chance of convincing the homeowner of the need to weatherize or retrofit. In contrast, we found that such a lack of interest on the behalf of the public was due to lack of knowledge and information, and that part of the function of a HERS should be to educate the public, increase their energy awareness, and create a demand for energy efficiency.

We found that the success in implementing a HERS is dependent on success in *marketing* the HERS. Successful marketing is achieved only after a

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings and Community Systems, Building Services Division, U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.

comprehensive appreciation and treatment of the diversity in target populations. Programs that have had a restrained approach to the implementation of HERS—by insisting on treating implementation problems as basically technical, engineering problems (e.g., focusing on the accuracy of the tool), or by taking a laissez-faire approach to marketing (e.g., simply meeting a demand for energy efficiency, rather than helping to create more demand)—or programs that have adopted an aggressive, non-responsive approach, have had a poor track record.

HERS that are actively marketed, have a comprehensive appreciation of the market, are adaptive to the needs of particular users, and include user participation in the operation and revision of the program, are more successful in terms of penetration rates and in improving the energy efficiency of the older housing stock. Where successful, HERS have penetrated an estimated 40% of the new construction market and 20% of existing construction, and energy savings have ranged from 10% to 50%. These savings do not take into account the impact of HERS on non-participants, so that HERS are more successful than indicated by the direct savings alone.

Home energy rating systems have been used effectively in the new housing market, influencing builder behavior through the institution of voluntary programs. Typically, HERS have been very successful in this regard, especially when two market criteria are met: (1) the HERS was introduced in a recessionary period, when builders are most receptive to novel ways of promoting their buildings, in ways that involve actual savings to future homeowners; and (2) the HERS is aggressively promoted by the HERS agency, with widespread media campaigns and much support of the builder, including cooperative advertising, and marketing materials and assistance.

For existing stock, the only valid measure of the success of a HERS involves consideration of the effective implementation of retrofits and weatherization activity. There are some HERS currently addressing existing homes, but the opportunity for more work in this area continues to be large. We believe that the key to such an effective implementation involves an authoritative measuring device that can be used to evaluate a building's current energy efficiency, as well as evaluate alternate ways of improving that energy efficiency. This evaluation should be capable of translation into cost-effective terms, which generally has the most significance to the average homeowner.

A further important key to the success of a home energy rating system involves the inclusion of the homeowner in the use of the tool, so that the homeowner is informed what might be done to his house, what this physically involves, and what the consequences will be in terms of energy, cost, and, very importantly, comfort. And we further feel that it is important to the success of a HERS to provide assistance to the homeowner to make such changes. This assistance should not simply take the form of zero or low-cost loans, but also information about local sources of materials and contractors to do the work. Educational programs, including workshops on how homeowners can do some of this retrofitting themselves, may also be of great benefit.

PLANNED ACTIVITIES FOR FY 1988

This research has been concluded and no further activities are planned.

SUGGESTED READING

1. Vine, E., et al. (1987), "Implementation of Home Energy Rating Systems," LBL-22872.

Federally-Assisted Housing: Progress and Plans*

R. Ritschard, C. Goldman, K. Greely, E. Mills, and E. Vine

The U.S. Department of Housing and Urban Development (HUD) is America's largest landlord and pays the largest residential energy bill—over $2 billion per year for all federally-assisted housing programs. Forty percent of low-income renters reside in public housing. Preliminary analysis of this sector indicates that a significant potential exists for improving the energy efficiency of its stock. However, these potential savings have not been fully realized for a number of reasons, such as lack of technical information on the effectiveness of various conservation measures, retrofit costs and paybacks, available financing mechanisms, and the perception that there are few incentives to conservation.

In FY 1985, the U.S. Department of Energy (DOE), as part of a multifamily retrofit research program, initiated an effort to improve the energy efficiency of the federally-assisted housing stock with initial emphasis on public housing. LBL, in its lead role in this sector, compiled background information on public housing buildings, their physical characteristics, energy use patterns, conservation potential, and barriers to energy retrofit activity. From this technical background data, we formulated a research agenda and multiyear plan that begins to address the perceived barriers to attaining the conservation potential in public housing.

To overcome the barriers in this sector, we followed several approaches. These include analysis of utility bill data for several years calculating weather-corrected consumption levels, compilation and analysis of building and energy consumption data for past and current retrofit activities, evaluation of financing and HUD subsidy policy alternatives, development of simplified analysis tools and other models for audit and retrofit evaluation, occupant surveys, direct monitoring of retrofit performance, and information networking.

To date, our studies of public housing have:

- Created a computerized *data base* on the physical, demographic, and energy characteristics of nearly 1800 public housing buildings, which represent 91 projects and approximately 32,000 dwelling units; utility bills include 1 to 5 years of data.
- Performed an analysis of available *baseline energy use* at 91 projects to develop energy use indices for different building types and locations (see Annual Report article in this section by Greely, *et al.*).
- Conducted systematic evaluations of existing utility billing data on pre- and post-retrofit activities at 43 selected public housing sites to determine the range of *energy savings* and found the median savings to be 14%; median payback was 12 years (versus 3 years in private multifamily buildings).
- Developed a methodology for examining the relative *financial impacts* on HUD and public housing authorities (PHAs) of different conservation investment strategies and applied it at two local authorities (San Francisco and Trenton) to test alternatives to current HUD policies, such as the Performance Funding System which was found to discourage maintenance, third-party financing, and the use of PHA surplus funds for energy conservation.
- Monitored *domestic hot water consumption* in four public housing apartment buildings and constructed a model of household water consumption based on tenant interviews.

ACCOMPLISHMENTS DURING FY 1987

In FY 1987, we conducted three major activities in support of the overall goal of improving energy efficiency of public housing buildings. First, we identified and assessed simplified analytical tools used to evaluate energy and cost savings of options in multifamily buildings. Since building practitioners are increasingly relying on microcomputer-based techniques (rather than on main-frame computer programs) because of their ease of use, speed, and cost, we limited our evaluation to four public-domain microcomputer programs developed with DOE support: ASEAM-2, CIRA, COSTSAFR, and PEAR.

Our assessment concluded that none of the DOE-sponsored programs evaluated meets the specific needs of in-field auditors, weatherization program designers or managers, or policy-makers involved with retrofit decisions for multifamily buildings. However, each program, individually, possessed one or more important feature required in retrofit evaluations. In addition to the public domain programs, we identified 27 other simplified

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings and Community Systems, Building Services Division of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.

methods developed by the private sector. We also concluded that a follow-on assessment of a subset of these private sector programs was needed to test their appropriateness for retrofit analysis in multifamily buildings.

A second major activity in FY 1987 was to develop a generic accounting program that tracks utility consumption and costs at the local housing authority level and assists in reducing utility costs. The overall goal of this task is to assist small, medium, and large housing authorities to increase their potential for additional energy conservation and operational efficiency. The utility accounting program, which is co-sponsored by HUD, can be directly used by both PHAs and regional HUD offices to explore opportunities for utility bill reduction and the need for additional maintenance.

This year, we completed a draft program that employs a menu-driven format for use with the Lotus 1-2-3 software package for IBM-compatible personal computers. The user each month enters raw consumption data on gas, oil, electricity, water, and "other" utilities, such as solar meter readings. As the year progresses, the program can provide estimates of year-end consumption and costs so that a housing authority can budget ahead. The program's output, which is both tabular and graphical, is suitable for use with special HUD reporting forms for utility accounting and annual performance funding requirements, as well as for utility reviews periodically submitted to HUD. A design of the program format, as a series of input and output screens, was sent to a panel of reviewers with representatives from DOE, HUD (both the national and regional offices), local housing authorities, and the technical community.

The third accomplishment was in the area of information networking and technology transfer. In FY 1987, we organized and participated in a workshop on "Overcoming Barriers in Public Housing" at the Affordable Comfort Conference (Pittsburgh). We also led a workshop at the annual convention of the National Association of Housing and Redevelopment Officials (New Orleans) on "Energy Conservation in Public Housing: What Have We Learned?". The participants at the New Orleans workshop represented various PHAs who had first-hand experiences on what has or hasn't worked over the past several years to reduce utility costs in the public housing sector. At each of these conferences, LBL's research results were exchanged with both the technical community and building practitioners from local housing authorities around the country. Articles on public housing issues were also written and published this year in the *Maintenance and Modernization Supervisor*, which is one of the major trade publications serving the federally-assisted housing sector.

PLANNED ACTIVITIES FOR FY 1988

Next fiscal year, we will perform several tasks in support of the federally-assisted housing study. They include: (1) complete the utility accounting program and test it at selected housing authorities; (2) update the retrofit analysis at 43 public housing projects in order to evaluate the persistence of savings over time; (3) prepare input, which is specific to public housing buildings, to the multifamily energy auditing methodology being developed by DOE; (4) evaluate utility data from HUD's Modernization Needs Study collected by Abt Associates; and (5) continue the technology transfer/information network activities.

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Determinants of Measured Energy Consumption in Public Housing*

K.M. Greely, E. Mills, C.A. Goldman, R.L. Ritschard, and M.A. Jackson

U.S. public housing currently shelters more than 3.5 million low-income tenants and accounts for 5.7% of the multifamily housing stock in this country. The program, which was initiated in 1937 with the passage of the U.S. Housing Act, is operated and managed by the U.S. Department of Housing and Urban Development (HUD). Annual energy costs now exceed $1 billion, which is 85% of the annual operating subsidies provided by HUD, or one-third of annual operating costs. Because energy expenditures are so high, they are a prime target for HUD's efforts to cut costs in response to tightening budgets. Our study describes a method for analyzing housing project energy consumption that HUD can use to establish energy-use guidelines and to evaluate public housing authorities' (PHAs) operating budgets.[1] Energy use indices such as those developed here can also help PHAs monitor their energy consumption and plan effective energy management strategies.

In this study, we analyze energy use in 91 selected public housing projects across the U.S. using both utility billing data and fuel oil consumption data. We believe this analysis represents the most comprehensive examination of energy consumption patterns in public housing based on *measured* data. After adjusting annual consumption for changes in weather, we examine correlations between energy use and building and occupant characteristics, using multiple regression analysis. Energy use and costs for different subgroups of our sample (for example, high-rise and low-rise buildings) are also characterized. In addition, we compare measured energy use in public housing with engineering estimates of public housing consumption, as well as with measured consumption in privately owned multifamily buildings.

The 91 selected projects are drawn from 19 local housing authorities and represent 1789 buildings and 31,928 apartments. All regions of the country are represented, although 70% of the projects are located in the Northeast. Most of the projects in our data base are located in climates that have between 4000 and 6000 heating degree-days. Only 13% are located in climates with relatively mild heating seasons compared to 44% of the public housing stock. Sixty% of the projects in this study are low-rise buildings (four stories or less), a slightly smaller percentage than within the total public housing stock. Almost 75% of the selected projects are centrally heated, a much higher percentage than in the total public housing stock (37%).[2] Gas is the most common space heating fuel in our projects, followed by oil, which is much more prevalent in our sample than in public housing in general (44% versus 13%). The selected sample has a significant number of senior projects (32%), which parallels trends in the overall stock.

ACCOMPLISHMENTS DURING FY 1987

This study utilizes a two-part model. In the first part, actual energy use is normalized to consumption in a year with "typical" weather, using the Princeton Scorekeeping Method, a widely used energy analysis model that finds weather-normalized annual consumption by regressing energy use versus degree-days calculated at the best-fit reference temperature. Then, in stage two, this normalized energy use is used to examine the influence of project characteristics on consumption levels, using multiple regression analysis.

We found that annual energy consumption of the space heat fuel (which includes domestic hot water and some cooking consumption) was 105 MBtu/apt. (129 kBtu/sq.ft.), while total fuel and electric consumption was 122 MBtu/apt. (158 kBtu/sq.ft.). Median energy (fuel and electricity) expenditures were close to $1000/apt. for this group of projects. Some interesting patterns emerged when the projects were separated by building type, heating system and fuel type, and type of occupant. Median energy consumption in the high-rise projects was 16 to 23% lower than for the low-rise projects, after we adjusted for floor area and the number of units, respectively. On average, the projects that heated with gas used 25% (per square foot) to 32% (per apartment) less energy than the oil-heated projects. The senior projects used 11% less energy than the family buildings, when adjusted for differences in floor area.

Projects in this study used 8% (per square foot) to 16% (per apartment) less fuel and electricity than previous engineering estimates of consumption for the public housing stock developed in the Ehrenkrantz report (a HUD-sponsored study assessing the physical condition of the public housing stock).[2] Non-heating electricity use was the same for both our projects and the stock estimates, while oil and gas consumption was 16% (per square foot) to 19%

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Building and Community Systems, Buildings Services Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

(per apartment) lower for our sample than that estimated in the Ehrenkrantz report. Lower consumption among projects in our sample may reflect the energy-conserving character of the PHAs that contributed data. Energy use per square foot in this group of projects is still significantly higher (74%) than in the privately owned multifamily stock. (See Figure 1.)

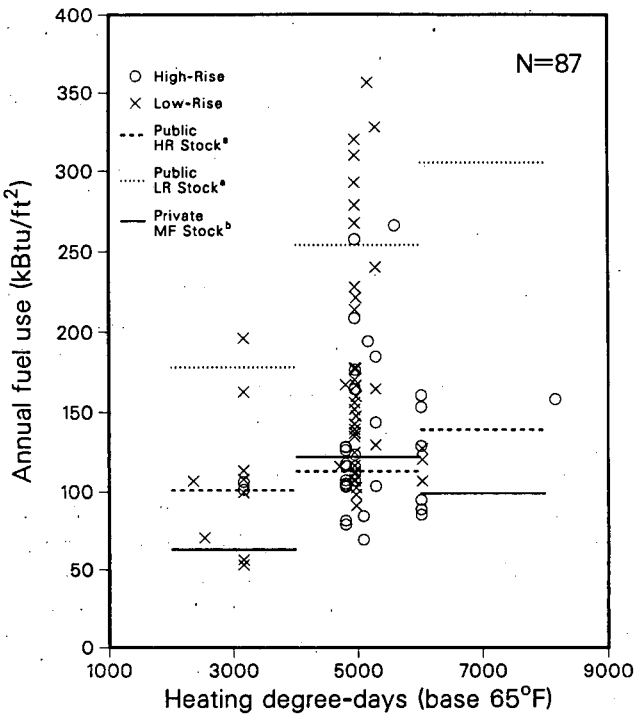

Figure 1. Comparison of consumption of space heat fuel with heating degree-days for different building types. Space heat fuel includes consumption for space heat, domestic hot water, and some cooking. Measured consumption at many projects is lower than engineering estimates of public housing stock use, but still significantly higher than private multifamily consumption. (XBL 8711-9090 A)

We developed two multiple regression models that were able to explain between 50% and 80% of the variation in fuel consumption in our sample of projects, using building and demographic characteristics and housing authority as independent variables. In these projects, occupant type was the most important factor that explained variation in energy consumption; projects occupied by seniors used less energy than family projects. The results of this analysis also suggest that the management practices of local housing authorities is an important determinant of energy use in these projects. We conclude that this two-stage methodology could be used to help HUD and PHAs increase their understanding of energy use patterns among projects and gain greater control of energy expenditures.

PLANNED ACTIVITIES FOR FY 1988

During the next year, we plan to apply this two-part model to a statistically representative sample of the public housing stock that is currently being compiled as part of a HUD-sponsored study. A regression model derived from this sample could give HUD a basis for developing PHA energy use guidelines that would take into account structural and demographic factors.

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Computer-Generated Residential Building Loads Data Bases*

J. Huang, J. Bull, and R. Ritschard

Large computer models for detailed building energy simulation such as DOE-2 are very useful for calculating the energy saving potential of various building conservation measures through repetitive simulations under consistent operating and climatic conditions. The resultant data base can be applied to the development of energy conservation standards, design guidelines, or simplified analysis tools.

Over the past decade, the Building Energy Analysis Group has conducted extensive computer analysis of the impact of conservation measures on residential energy use in different U.S. locations. From 1982 to 1986, we compiled a large data base of residential energy use using the DOE-2.1A and DOE-2.1B programs. The technical documentation for this effort is in a LBL report[1], while the data has been incorporated into the PEAR (Program for Energy Analysis of Residences) microcomputer computer program.[2]

In 1987, we were asked by Pacific Northwest Laboratories (PNL) to create a new version of this data base for a microcomputer-based residential energy standard PNL was developing in conjunction with ASHRAE, with support from DOE. We substantially reduced the effort required for this task by utilizing regression techniques developed from our earlier work. This allowed us to produce a data base that was compact, analytical, and flexible. Although the data base is presented in various ways, the primary output are sets of regression equations that comprise a simplified technique to estimate energy use in typical houses of varying sizes, shapes, and conservation levels.

ACCOMPLISHMENTS DURING FY 1987

The new data base was generated during FY 87 using a enhanced version of the DOE-2.1C program. The simulations cover three prototype buildings (one-story, townhouse, and apartment) in 45 U.S. locations. For each prototype and location, three foundation conditions (slab-on-grade, basement, and vented crawl space) and a range of insulation, wall mass, infiltration, and window options were considered. The changes in annual heating and cooling loads due to these building variations were analyzed through regression techniques, and reduced to generalized functions relating to the thermal and physical characteristics of the building components, e.g., areas and U-values for ceilings, walls, and floors, plus solar aperture and orientation for windows, or effective-leakage-areas for infiltration (Figure 1).

The methodology for the new data base is based on our earlier work[3], but incorporates recent advances in modeling abilities and analysis techniques. In addition to the improved algorithms resident in DOE-2.1C, enhancements were made to the code to model two-dimensional heat flow through walls and underground surfaces, and more realistic window operations for shading and natural ventilation. A quadratic regression with five variables, four for window solar apertures in each orientation and one for total solar gain, was found to produce reliable estimates of energy savings for different window conditions (Figure 2).

To account for two-dimensional heat flow in walls, we developed a finite-element program, WALFERF, to calculate response factors for two-dimensional heat conduction. In addition to specifying the thermal properties, thicknesses, and sequence of materials making up each block, WALFERF also requires the number of blocks and their widths.

Since the standard DOE-2 program does not adequately model the building-to-ground interface, we worked with the Underground Space Center (USC) at the University of Minnesota to incorporate into the DOE-2 program heat fluxes calculated by a two-dimensional finite difference program developed at

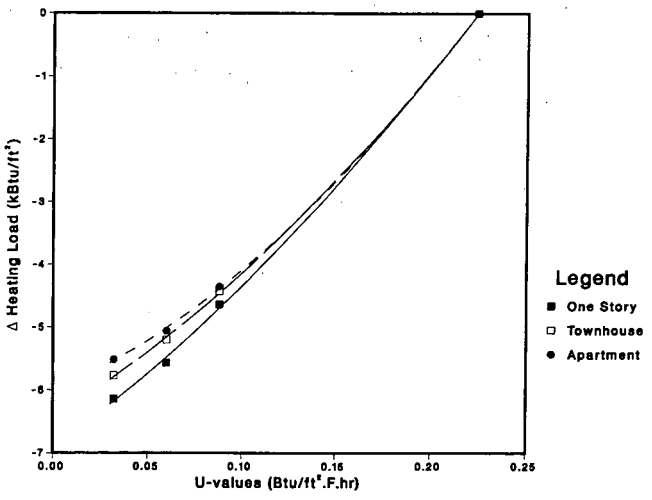

Figure 1. Correlations of Δ wall heating loads to U-values for Phoenix. (XBL 8711-4982)

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings Energy Research and Development, Building Systems Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, through Battelle Pacific Northwest Laboratory.

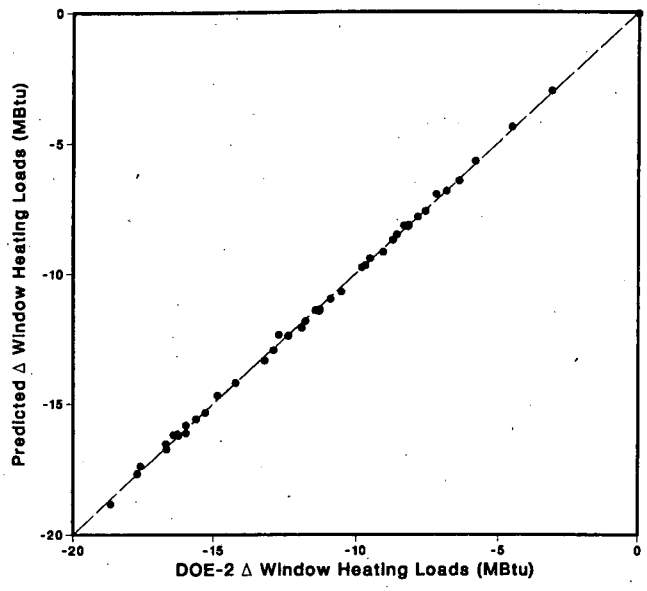

Figure 2. Quadratic correlation of Δ heating loads to solar aperture times solar usability in Albuquerque. (XBL 8711-4985)

Albuquerque NM WYEC One Story Prototype Siding

Heating Load

Ceiling	Delta (MBtu)	Component (KBtu)	(/sf)
R-0	.00		22.58
R-7	-21.01		8.94
R-11	-24.37		6.76
R-19	-27.38		4.81
R-22	-28.52		4.07
R-30	-30.05		3.07
R-38	-30.97		2.47
R-49	-31.77		1.96
R-60	-32.28		1.62
Slope(DD)		4468.29	
Curve(DDS)		-111.142	

Wall	Delta (MBtu)	Component (KBtu)	(/sf)
R-0	.00		19.81
R-7	-11.65		9.44
R-11	-13.31		7.96
R-13	-15.32		6.18
R-19	-16.31		5.29
R-27	-17.95		3.84
R-34	-18.95		2.95
Slope(DD)		3773.11	
Curve(DDS)		-16.709	

Slab			(/ft)
R-0		-16.12	39.78
R-5	2ft	-19.37	20.20
R-5	4ft	-19.96	16.64
R-10	2ft	-20.01	16.34
R-10	4ft	-20.81	11.52
Intercept		.000	
Slope(DD)		4155.71	
Curve(DDS)		-.186	

Heated Basement			(/ft)
R-0		-8.95	82.97
R-5	4ft	-14.13	51.76
R-5	8ft	-15.20	45.32
R-10	4ft	-15.42	43.99
R-10	8ft	-17.02	34.35
Intercept		9.144	
Slope(DD)		2834.65	
Curve(DDS)		-22.466	

Figure 3. Sample data base; tabular output. (XBL 8712-5165)

the USC to simulate below-grade heat flow. This procedure captures the seasonal thermal behavior of the underground surface with its enormous thermal mass and heat capacity (see accompanying Annual Report article on foundation insulation modeling).

The data base is presented both as tables giving the Δ load for incremental changes in conservation level, or more analytically as regression coefficients expressing the Δ loads of each building component as a function of its physical and thermal characteristics. Figure 3 is a sample of the data base tables in the technical report[4]. The columns give the Δ loads for various insulation levels from the uninsulated base case, while the "slope" and "curve" give the quadratic and linear regression coefficients for the component load as a function of total ceiling or wall conductance.

PLANNED ACTIVITIES FOR FY 1988

The analytical format of the new data base makes it a flexible tool for calculating energy use in typical residential buildings. In FY 1988 we hope to incorporate the new data in the PEAR microcomputer program, and develop further the analytical approach used for both the DOE-2 simulations and the results analysis. We are also planning to analyze in more detail interactions between different building components, notably those affecting building cooling loads such as ventilation rates and thermal, and those relating to window solar gain.

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Conservation Potential of Foundation Insulation Measures*

J. Huang and J. Bull

In the last decade, there have been significant improvements in the thermal integrity of new houses through increased use of ceiling and wall insulation, multiple-pane windows, and reduced infiltration. Current building practices, however, often ignore foundation insulation because of uncertainty about their potential benefits. Although measured data have indicated that the conservation benefits may be large, there is need for a systematic study of the thermal performance of different foundation options.

In FY 1987, the Building Energy Analysis Group worked on a DOE-funded project headed by the Underground Space Center (USC) at the University of Minnesota to develop a handbook on energy-efficient building foundation design.[1] The purpose of the handbook is to provide design guidance to architects and designers on residential foundations with emphasis on energy and structural issues. LBL's role in the project was to develop with the USC a procedure for simulating the energy uses of a typical residential building with nearly 90 different foundation conditions for 13 U.S. locations.

ACCOMPLISHMENTS DURING FY 1987

The energy performance of a building foundation is difficult to simulate due to the thermal coupling between the building and the surrounding subsoil. Whereas light-frame walls respond thermally to temperature changes within a few hours, and even a massive wall within a day or two, the thermal responses of foundations extend over months or even years.

The procedure developed jointly by LBL and USC was to combine the capabilities of a finite-difference program at USC to simulate below-grade heat flows with that of the DOE-2.1C program at LBL to simulate whole house performance. The USC model is a fully-implicit integrated finite difference heat conduction program that provides a detailed two-dimensional heat flow simulation for the foundation and subsoil. The use of DOE-2.1C provides a hourly simulation of the rest of the house with realistic operating conditions, as well as compatibility with previous data base work done at LBL (see accompanying Annual Report article on residential loads data base). For foundations with floating zone temperatures such as unheated basements and crawl spaces, we developed an iterative procedure alternating between the two programs to capture adequately seasonal variations in the below-grade heat flux due to the heat storage of the soil.

We used the USC model to simulate on a daily time-step the heat flows in a representative one-foot vertical section of the foundation and surrounding soil (Fig. 1) under three conditions: 1. the same constant indoor temperatures as used in DOE-2 Loads, 2. a different constant indoor temperature, and 3. a series of sinusoidal varying indoor temperatures of different amplitudes. We then integrated these heat fluxes over the "footprint" of the prototype foundation to derive the average hourly fluxes each day through the underground surfaces of the prototype buildings (Fig. 2).

The fluxes calculated with the first condition are substituted for the standard heat flow calculation for underground surfaces in DOE-2 Loads. The fluxes calculated with the second condition are used to derive steady-state conductances for the foundation, while those calculated under the third condition are used to derive the periodic changes in heat flows due to seasonal variations in the indoor temperature:

$$Q_{\text{Loads T}} + \Delta Q_{\text{constant }\Delta T} + \Delta Q_{\text{sinusoidal }\Delta T}$$

For unconditioned spaces such unheated basements and crawl spaces, there are large seasonal fluctuations in the zone temperature, and hence large

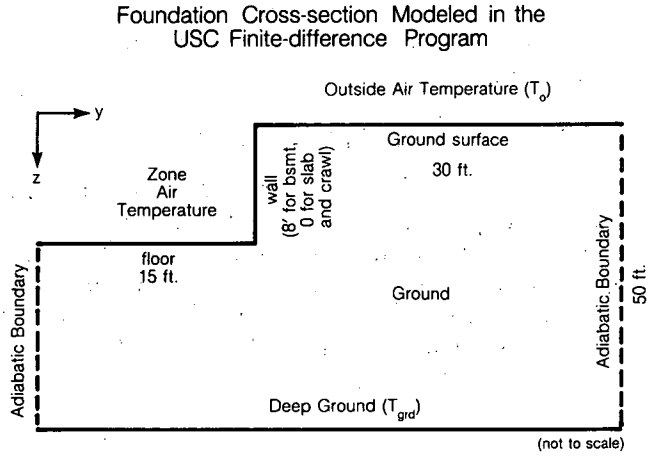

Figure 1. Foundation cross-section modeled in the USC program. (XBL 8711-9360)

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings Energy Research and Development, Building Systems Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, through Oak Ridge National Laboratory and the University of Minnesota.

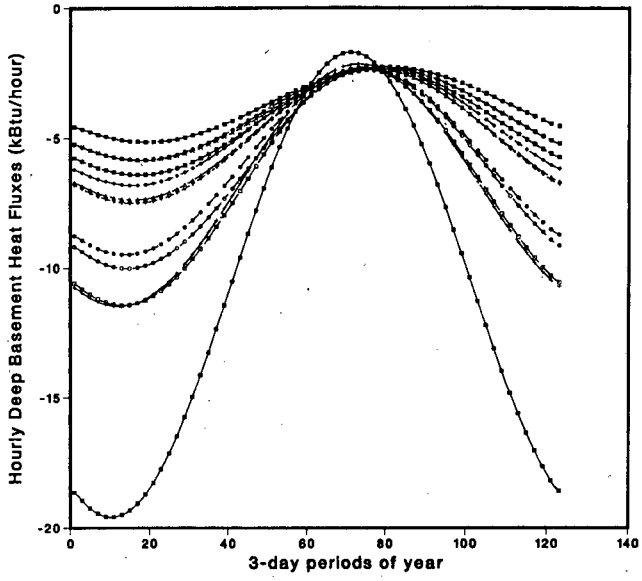

Figure 2. 70°F temperature fluxes for various deep basement foundations in Minneapolis, MN. (XBL 8711-4984)

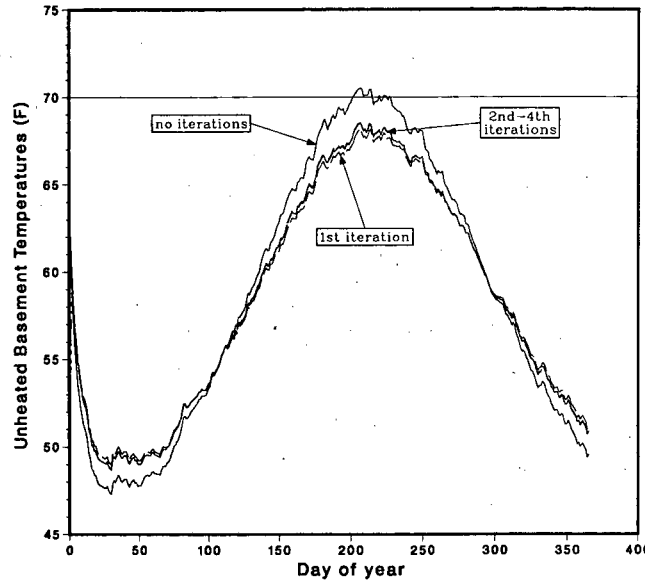

Figure 3. Floating temperatures in an uninsulated basement in Minneapolis, MN, after 5 iterations. (XBL 8711-4983A)

dynamic flux modifications for changes in indoor temperatures ($\Delta Q_{sinusoidal\ \Delta T}$). Since the zone temperatures are outputs from the DOE-2 simulations, we developed an iterative procedure using the zone temperatures from the preceding DOE-2 run to determine the $\Delta Q_{sinusoidal\ \Delta T}$ for each subsequent simulation. We found that by alternating between the USC model and DOE-2.1C, we achieved convergences in the computed zone temperatures and building energy uses by the fourth iteration (Fig. 3).

By the end of FY 1987, we have completed half of the 1300 required simulations. The results will appear as tables in the foundation design handbook showing the changes in annual heating and cooling energies from base case foundations with no insulation. In addition, the handbook includes an economic analysis that compares these energy savings to construction costs and develops design guidelines.

PLANNED ACTIVITIES FOR FY 1988

The data base is scheduled for completion before the end of 1987, and the handbook by early 1988. In addition to completing the data base for 89 foundation types in 13 cities, we will also perform sensitivity analyses on the impacts of different soil conductivities and snow cover on the energy savings of foundation conservation measures. To document the methodologies used in our energy simulations and economics analysis we are planning to present three technical papers at the ASHRAE Summer 1988 conference in Toronto.[2,3] By that time, we also hope to have completed comparisons of our results to available measured data and results from other simulation efforts.

Although at present we are only using the results from DOE-2 for total annual heating and cooling energy use, the data also includes a wealth of information on monthly and peak loads, and zone temperatures. Both USC and LBL are interested in improving our modeling capabilities and developing useful applications of the data.

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BUILDINGS ENERGY DATA

Overview

The Buildings Energy Data Group (BED) compiles and analyzes measured energy performance data on buildings and equipment. The Group's goal is to identify building design strategies and end-use technologies that save energy or modify electrical loads, and are cost-effective. We provide these measured results to institutions and persons responsible for improving energy efficiency in the buildings sector. In addition, we use the data to estimate regionwide potential savings from energy-efficient technologies.

The core of BED's activities rests in the Buildings Energy-Use Compilation and Analysis (BECA) series. Each data compilation addresses a sector of the buildings end use:

- New, low-energy homes (BECA-A)
- Retrofits of existing residential buildings (BECA-B)
- New, energy-efficient commercial buildings (BECA-CN)
- Retrofits of existing commercial buildings (BECA-CR)
- Residential water heating systems (BECA-D)
- Validations of computer loads models (BECA-V).

Each compilation is an independent data base, but all rely on the same computerized data base management system (DATATRIEVE). Each data base can be queried so as to produce buildings with similar features, location, function, etc. The article by Goldman and Greely on multifamily retrofits (a subset of BECA-B) is an example of the compilations developed by the Group. In another sub-compilation, Piette and Wyatt assessed the measured energy performance of cool storage systems in commercial buildings.

An important research goal of the BED Group is to develop, refine, and promote the wider use of standard "yardsticks" of building energy performance. For automobiles, a dynamometer test yields a single parameter of fuel efficiency (miles per gallon). Unfortunately, one cannot measure a building's energy use under similarly controlled conditions. Instead, we must collect detailed information about the building, including its energy consumption, physical characteristics, and operating schedule. This information permits us to convert "raw" measurements into standard energy performance indicators. In the past, indicators focused on energy savings and cost-effectiveness; we are now developing parameters that describe peak power savings or, more generally, reshaping of electrical demand profiles.

The BED Group is also active in two areas that complement the core data compilation effort: primary data collection and conservation potentials studies. In special circumstances, BED measures energy use in specific buildings or equipment. This usually occurs after we have identified significant gaps in available data or collection techniques. The article by Akbari *et al.* describes measurements of the higher temperatures caused by the urban heat island. In another study, we tapped in-place energy monitoring systems to demonstrate that valuable commercial building performance data could be obtained quickly and cheaply. We also participate in monitoring projects or analysis of primary data. The article by Meier and Nordman describes the incremental value of metered data in an analysis of energy savings from new building standards.

Measured data on energy use and savings are key inputs to least-cost utility planning. The BECA compilations provide a valuable data base from which to estimate the potential for energy efficiency and electric load-shaping. The BED group has undertaken numerous investigations of the potential energy savings in the buildings sector. The potentials studies typically examine a series of end-use measures, calculate the costs of conserved energy, and develop "supply curves of conserved energy" (or peak savings) to express the aggregate potential for end-use efficiency. The article by Krause describes how we developed supply curves of conserved electricity (and load shape impacts) for Michigan. Related activities include the development of improved, microcomputer-based software to simplify the assessment of energy efficiency potentials. This software will be linked to a data base on end-use technology characteristics—much of which originates from our BECA research—containing data on measured energy use, savings, costs, and related technical issues.

An Updated Compilation of Measured Energy Savings in Retrofitted Multifamily Buildings*

C.A. Goldman and K.M. Greely

The multifamily sector, consisting of residential buildings with two or more units, comprises almost 27 percent of the U.S. housing stock (in terms of household units). Annual site energy use in these buildings is approximately 2.3 quads (1 quad = 10^{15} Btu) and directly or indirectly costs U.S. households almost $20 billion.

We have compiled and analyzed measured data on 200 U.S. retrofit projects in existing multifamily buildings that are now part of the Buildings Energy Use Compilation and Analysis (BECA) residential data base. We examined the costs of conservation measures and practices and the savings they generate. In this article, we also discuss the cost-effectiveness of different retrofit strategies in fuel and electrically heated buildings.

We obtained information on retrofit projects from several sources, including city energy offices [70], public housing authorities [38], research institutions and national laboratories [17], non-profit and for-profit energy service companies [36], and utilities [39].† During the past year, 40 electrically heated buildings from the Pacific Northwest have been added to our compilation. The data collected typically included metered energy consumption, installed retrofit measures and their costs, the price of the space heating fuel the winter after retrofit, and a brief description of the physical characteristics of the building. In most cases, we (or our data source) used the Princeton Scorekeeping Method (PRISM) to analyze energy consumption data before and after retrofit. PRISM estimates a weather-normalized annual energy consumption (NAC) from parameters obtained from a regression of either utility bill or meter readings of the space heat fuel and daily average outdoor temperature. The NAC represents consumption that would occur in a year with typical weather conditions.

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings Energy Research and Development, Building Systems Division of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.

†Numbers in brackets represent number of data points obtained from each source.

ACCOMPLISHMENTS DURING FY 1987

Median annual energy savings for our group of buildings were 9 MBtu per dwelling unit, or 16% of pre-retrofit energy use. Fuel-heated buildings saved more absolute energy, but percentage savings are similar in both groups (17% vs. 14%). We have found that energy savings are between 10 to 30% of pre-retrofit energy use in 60% of the buildings in our compilation. The median payback time for electrically heated buildings is over 20 years, while those of privately owned and public fuel-heated buildings are 4 and 10 years, respectively. In most cases, it is not cost-effective to spend more than $1500/unit.

The kind of retrofits implemented in a building depend mainly on the type of energy used for space heating. In fuel-heated buildings, various HVAC system retrofits (heating controls, equipment replacement, and altered operation and maintenance practices) and domestic hot water system alterations are the most popular conservation strategies. Shell measures (insulation, weatherization, and window modification or replacement) are more commonly implemented in electrically heated buildings. Retrofit costs are less than $250/unit in 35% of the buildings; median costs for heating system retrofits were much lower than costs for shell retrofits ($150 vs. $1350/unit).

The most cost-effective strategies in the fuel-heated buildings were heating controls, especially outdoor reset and cutout controls, and balancing of single-pipe steam systems. Heating system replacements and conversions (e.g., high-efficiency boilers, separate domestic hot water generators, and distribution system conversions) have somewhat longer payback times (5 to 20 years), but resulted in substantial savings (15–30%), as illustrated in Figure 1. The shell and window measures common in electrically heated buildings had payback times of about 20 years, with savings of 14 and 11%, respectively (Figure 2). Almost all of the electrically heated buildings in our compilation were retrofitted as part of utility programs with high investment levels; program economics could be improved by targeting high users (many electrically heated buildings have very low pre-retrofit consumption levels) and focusing on less expensive lighting and domestic hot water retrofits.

PLANNED ACTIVITIES FOR FY 1988

We are investigating the stability of savings in buildings during the years following a retrofit. Preliminary evidence suggests that substantial changes in consumption, both positive and negative, can occur between the first and second year after retrofit. Dur-

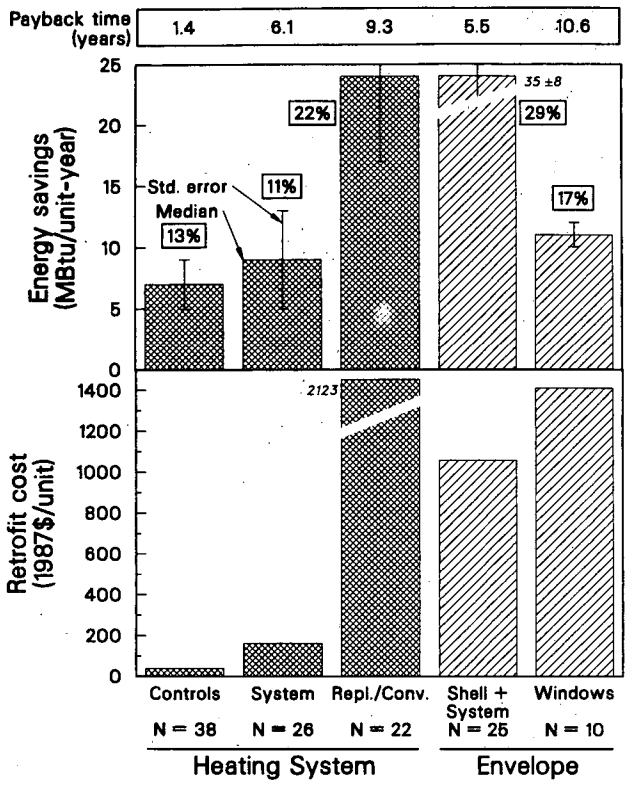

Figure 1. Energy savings and costs of retrofits in fuel-heated multifamily buildings. "System" refers to groups of measures that affect the heating or hot water systems. "Repl./Conv." are replacements or conversions of the boiler/furnace or distribution system. "Shell + System" includes combinations of retrofits which reduce heat loss through the building shell, and measures affecting the heating or hot water systems. (XCG 8710-14122).

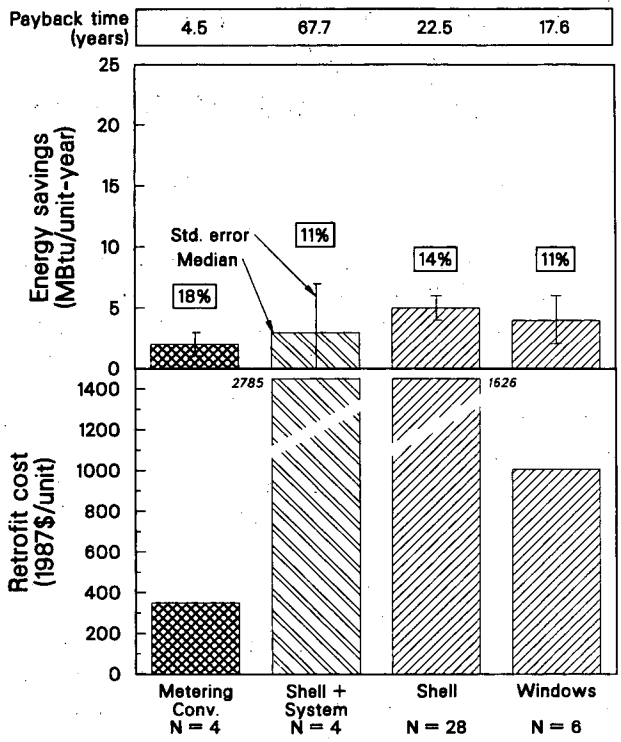

Figure 2. Energy savings and costs of retrofits in electrically heated multifamily buildings. "Metering Conv." are conversions of a master-metered billing system to one with individual apartment submeters. "Shell" refers to combinations of retrofits which reduce heat. (XCG 8710-11421)

ing the coming year, we will obtain additional post-retrofit consumption data for as many of the retrofits in our data base as possible, to increase our understanding of the building and retrofit characteristics which influence the persistence of savings.

Another activity during FY 1988 will focus on estimating the energy savings potential of the U.S. multifamily stock by extrapolating from the measured data in the BECA residential data base. Using data from the Energy Information Administration's Residential Energy Consumption Survey, we will compare characteristics of the U.S. stock with those of buildings in our compilation, to see what kinds of retrofits would be applicable to the stock, and how much savings could be expected if these retrofits were implemented.

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Incremental Value of Measured Data from the Residential Standards Demonstration Program*

A. Meier and B. Nordman

In an attempt to reduce future electricity needs, the Bonneville Power Administration (BPA) proposed to implement stringent efficiency electricity standards for new, electrically heated houses. BPA first sought to determine the potential energy savings for houses built to the Model Conservation Standards (MCS) through a major monitoring program. The Residential Standards Demonstration Program (RSDP) sponsored the construction of over 300 houses built to the MCS and selected over 300 recently-built houses to serve as controls. BPA asked LBL to estimate the actual energy savings from the MCS. A simple comparison of energy use was not possible because the houses differed greatly in their design and operation. Moreover, BPA sought to determine the energy savings under "normal" conditions to permit comparisons with its simulations of prototype houses. We applied techniques developed to support our compilation of new, low-energy homes (BECA-A) to analyze the savings. In particular, the program, SUBMET, normalizes metered space heating energy for differences in floor area, internal gains, inside temperatures, and climate.

We relied on weekly energy and temperature data from the triple-meters (which monitored space heating, water heating, and appliances) and temperature loggers. We also drew upon surveys and audits to provide floor areas and occupancy data.

MCS houses typically used 45% less space heat than Control houses (see Fig. 1). The regionwide savings were about 3.5 kWh^2-yr, but vary with climate zone. The estimated savings change when the assumptions are modified for internal gains and inside temperature. Most reasonable sets of assumptions yield annual savings over 3 kWh/ft^2-yr. The most sensitive assumptions are the choice of standard internal gains and the fraction of appliance energy that is converted to useful heat.

*This work was supported by the Bonneville Power Administration through the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

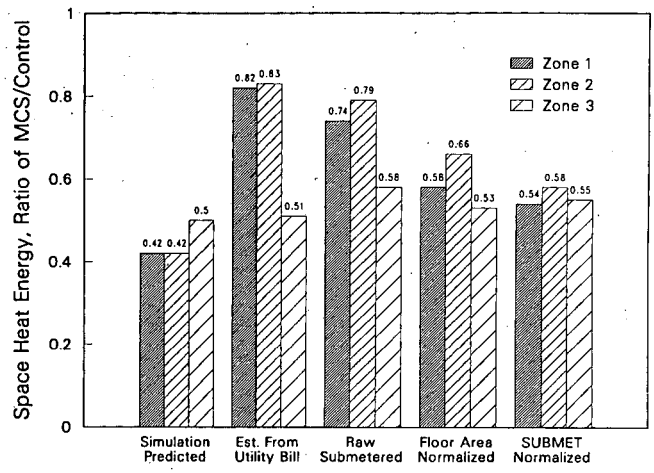

Figure 1. Five indicators of MCS/Control space heat energy. Each column represents the ratio of average space heating energy for MCS homes to their counterpart Control homes. A ratio of 1 would indicate that two groups used the same amount of space heat, while a ratio of 0.42 would indicate that the MCS houses used only 42% as much as the Controls. Differences in the groups disappeared as adjustments for more factors were incorporated. (XBL 8712-5274)

ACCOMPLISHMENTS DURING FY 1987

A program to monitor the energy use of buildings is expensive and time-consuming. Nevertheless, such information is essential to energy forecasters and planners because the costs of surplus capacity—or a shortfall—are even more expensive. We have focused on the incremental value of monitored data in assessing energy performance of buildings. Our goal was to determine the improvement in accuracy resulting from additional data collection.

Simulations always play an essential role in a comprehensive monitoring program. The simulations may consist of simple heat loss calculations or computer models to predict energy use and savings. BPA estimated the energy savings from the MCS for prototype houses compared to current construction practice. The simulations also determined the most cost-effective package of conservation measures. These predictions (shown in Fig. 1) predicted that the MCS houses would use less than half of the heating energy used by houses built to current practice.

The success of a program is often judged on the basis of monthly utility bills. By this measure, the MCS homes used about 17–49% less total energy. The savings in climate zones 1 and 2 are not surprising because the utility bill includes non-space heating

end uses, such as water heating and lighting, but the fraction of total savings for houses in climate zone 3 is very close to that predicted for space heating alone. This behavior cannot be explained with a utility bill analysis.

A comparison of space heating energy alone causes the savings in the three climate zones to converge. This comparison requires a second meter on the house and typically costs a few hundred dollars. In this case, the additional information changes results slightly.

A simple improvement can be obtained by adjusting each house's space heating use to reflect its floor area. When this is done, the MCS houses in all of the climate zones save 34–42%. The disparities among the climate zones are much smaller, and all zones are achieving savings closer to those predicted by the simulations. Much of the apparent difference in energy use was due to MCS houses being larger than the Control houses. The combination of space heating and floor area data greatly improved the accuracy of the results and explained the discrepancies found with utility bills alone.

Finally, we used SUBMET to normalize the measured space heating use so as to approximate the operating conditions used in the simulations. SUBMET adjusts for climatic differences (within each climate zone), floor area, inside temperature, and internal gains. After these adjustments, it appears that MCS houses used 42–45% less space heat than the Controls. The enormous differences among the climate zones virtually disappeared after accounting for differences in internal gains and indoor temperatures.

The MCS still did not achieve the energy savings predicted by the simulations. Both technical and behavioral factors may explain the (relatively small) difference. Control houses were better insulated and had lower measured infiltration rates than assumed in the simulations. In addition, the occupants operated the houses differently than assumed in the simulations. There is also considerable variation within the sample, so that the ratios predicted by the simulations are within the range of high statistical confidence. Alternatively, SUBMET may provide a biased estimate because it normalizes inside temperature based on only one indoor temperature. If the occupants practiced zone heating, a bias might be introduced.

We will test the zone heating hypothesis by tapping a richer data set on a smaller group of RSDP homes where multiple temperature sensors were installed.

PLANNED ACTIVITIES FOR FY 1988

We will develop statistical indicators to compare temperature deviations to permit a quantitative assessment of their differences. In addition, we will examine houses with unusually high and low space heating needs, and try to explain them in terms of the building characteristics and occupant behavior. Finally, we will compare the energy performance of the houses in the RSDP to those houses already in our BECA-A data base.

Analysis of Utility Program Experience: Preliminary Results from the MEOS Study*

F. Krause

The Building Energy Data Group has been expanding its work on technology cost and performance assessments to include experience with utility incentives programs to promote customer efficiency investments and participation in load management. A preliminary analysis of several appliance, lighting efficiency, and load management programs in the residential sector was performed as part of LBL's contribution to the Michigan Electricity Options Study (MEOS).

It is widely recognized that the implicit economic decision-making in the purchase of energy-consuming devices by energy consumers does not follow lines of least-cost rationality. One objective of the MEOS demand-side analyses was to define the amount of energy and peak demand savings that could be realistically obtained from the technologies considered, if utilities were to *aggressively* pursue specific incentive programs to shift the purchasing behavior of their customers. This requires incorporation of achievable annual participation rates and cumulative penetration fractions

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into the analysis. Also, the administration and incentives cost of such programs must be ascertained. Such an analysis is presently difficult because only a limited number of programs have been carefully monitored over an extended period of time, and even fewer programs have been aggressively pursued.

ACCOMPLISHMENTS DURING FY 1987

Our method was to assume that aggressive programs would provide incentives in such a way as to eliminate all extra first costs for participants (full incentives). High incentives alone do not guarantee high participation rates, but they do make participation less sensitive to non-financial program features. Programs also have to observe a number of lessons that emerged from a review of the literature and from interviews with program managers. Among these are:

- Large-scale programs should be preceded by well-designed and thoroughly evaluated pilot and demonstration projects.
- Monitoring, feedback, and quality control functions should be built into the implementation process.
- Programs should make use of market segmentation techniques and other methods to flexibly target different consumer groups and local conditions.
- Community groups and trade allies can be one of the most effective agents in the implementation process.
- Promotion of demand-side measures should emphasize how such measures contribute to the broad values sought by customers, such as increased comfort, safety, reliability, environmental health, and productivity.
- Information and incentives strategies should build upon market forces wherever possible, and reward savings rather than expenditures.
- Efficiency standards can be one of the most effective complements to incentives-based programs.

The program-based scenario in the LBL study assumes that full incentives are offered until most or all existing stocks have been turned over. The scenario also foresees for each end-use a *two- to five-year pilot project phase* in which program designs are optimized before full-scale implementation begins. The onset of major savings is correspondingly delayed.

The impact of increasing incentives on penetration fractions is schematically illustrated in Fig. 1, which shows the cost of conserved energy or peak power based on the sum of technology costs and costs for program administration (processing of rebates, advertising, etc.), for a stylized two-measure supply curve.

Two issues in calculating the cost of program-based demands-side resources are the free rider and spill-over effects of the program. In most cases, variable incentives based on careful analysis of existing purchasing patterns can minimize the free-rider problem. Spill-over effects are harder to quantify than free riders, but they will also counteract the free-rider problem. In a well-designed rebate program the spill-over effect can be made to dominate and provide program-induced savings from non-participants at zero program cost.

Another important variable in the utility cost of demand-side resources is the level of incentive that is needed to achieve desired levels of customer participation. Utility experience shows that substantial participation can be achieved at significantly less

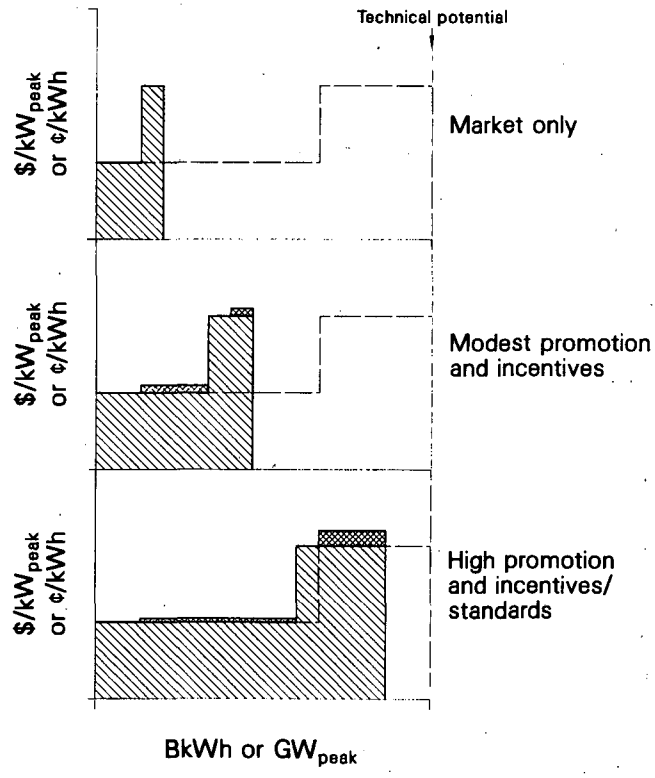

Figure 1. Technical potential and program-based scenarios: Costs of savings to society. (XCG 868-7347)

than full incentives. Utilities have also found that as programs mature, the level of incentives can be lowered and in some cases entirely substituted by effective information and promotion. This is partly the result of the programs' spill-over effects on the retail markets, such as better informed salespeople and greater stocking of high efficiency merchandise. Another reason is that in the larger utility incentives programs, the prices of demand-side technologies tend to drop as the program moves them out of their small, specialty or high-income market niche, where dealer mark-ups are high.

Since in our program scenario full incentives are provided over extended periods of time (eight to 15 years), the program costs developed in the LBL MEOS study define an upper bound for the likely cost of buying efficiency from customers.

PLANNED ACTIVITIES FOR FY 1988

We expect to prepare program experience reports on utility programs to promote efficient new construction practices and efficient commercial and residential lighting technologies.

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Technology Assessment: Cool Storage In Commercial Buildings*

M.A. Piette and E. Wyatt

In the last five years, utilities and state agencies throughout the country have sponsored programs to encourage better energy efficiency and load management in buildings. One promising load management technology is thermal storage for cooling commercial buildings. Commercial space cooling currently accounts for about 20 to 40 percent of most utilities' summer peak demand, and the Electric Power Research Institute estimates that commercial cool storage systems could avoid 17 GW of U.S. summer peak demand by the year 2000. The basic approach is to reduce on-peak demand (kW) by shifting the compressor's operation to off-peak hours, when electricity charges are lower. Cooling energy is stored in the evening using a medium such as water or ice, to be used the next day during occupied hours, which coincide with higher peak-period utility rates.

Commercial cool storage is not a new technology, but its widespread application in today's commercial buildings has required new developments. Most important are improvements in equipment and changes in operating strategies for various load conditions to optimize cost effectiveness under today's electricity rate schedules. About 200 new cool storage systems were installed in 1986, about double that of 1985; a similar doubling in 1987 is anticipated. The majority of systems are found in new office buildings, because they have low cooling requirements in the morning followed by high afternoon peak demands. Installations are most common in areas where utilities charge high demand rates or there is a high differential between day and night electricity rates. More than 20 utilities currently also offer direct rebates for cool storage, based on the estimated shifted peak demand (kW).

ACCOMPLISHMENTS DURING FY 1987

During 1987, we studied the current status and future potential of commercial cool storage.[1,2] There is clearly no single "best" system because the parameters, i.e., building type, load profile, status of existing equipment (if a retrofit or addition), first costs (considering any utility incentives or tax incentives), and electricity rate structures, strongly influence the design. Research and development is underway on more efficient refrigeration systems, ice building and storage techniques, and advanced phase change materials. Until recently cool storage has been used mainly in larger buildings with central chilled water systems. Now, a few manufacturers are offering packaged unitary rooftop air conditioning units with

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Building and Community Systems, Building Systems Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

ice storage. It is estimated that package units represent nearly three-fourths of the installed capacity for 1985.

Determining the cost-effectiveness of a cool storage system requires a comparison with a base case cooling system. Most cool storage systems are more expensive than conventional HVAC systems. The base case for an existing building is usually the "pre-retrofit" conditions. But comparison of "pre-" and "post-retrofit" building performance must consider any other changes in the building in addition to the installation of a cool storage system, which may be difficult. The base case for a new building is based on a "conventional" system. Performance analysis for a new buildings is, therefore, very sensitive to the specified characteristics of the "conventional" system. The most precise performance comparisons are based on actual metering of cooling loads. Measured cooling loads can then be used to calculate how a conventional system would perform under the same conditions that the cool storage system operated. Use of measured data accounts for the differences in weather and occupancy that occur between actual and simulated (or design) conditions.

Many cool storage buildings dramatically improve over the first few years. Figure 1 demonstrates the value of submetered cooling data in assessing the success of the cool storage system. While the average of the monthly on-peak demands for the cooling system fell from 1982 to 1985, the whole-building on-peak demands remained fairly constant.

Early cool storage installations experienced a number of startup problems. For example, many early systems were sized improperly. Table 1 summarizes the operating experiences for ten buildings. Sizing errors, control failures plagued many of the buildings. Inexperience of building operators was cited as a problem for six of the buildings. In almost every case system performance improved over the first few years as experience with the equipment and building operation was gained.

Standardized techniques for performance analysis have not been developed because the choice of relevant physical performance parameters depends on the rate schedule. Furthermore, both designers and building operators require training. Better estimates of cool storage potential require more detailed

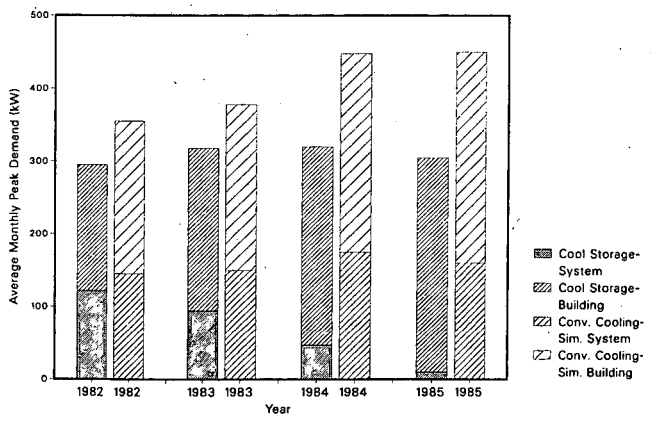

Figure 1. Average of monthly demands for an office building in the midwest USA for the whole building and for the cooling system alone during on-peak periods in four successive cooling seasons. As the operators mastered the cool storage system, they significantly reduced the average monthly demand. "Sim" and "Conv" refer to simulated and conventional, respectively. The simulated energy use grew in part due to the installation of a computer center. (XBL 8712-5275)

Table 1. Summary of Early Operating Experiences for Ten Buildings.

	Occurrences
SYSTEM DESIGN	
storage sizing	4
compressor sizing	2
condenser sizing	1
refrigerant receiver	2
water flow inadequate	1
storage poorly insulated	1
SYSTEM O & M	
control strategy unsatisfactory	1
improper expansion valve settings	2
time clock malfunctions	6
compressor failure	3
compressor control failure	3
refrigerant leaks	4
storage leaks	2
inexperienced maintenance personnel	6
inexperienced outside contractors	5
poor sensor calibration & maintenance	3
insufficient cooling on hottest days	1
excessive storage during mild weather	4
CHILLED WATER SYSTEMS	
poor tank stratification	2
ICE SYSTEMS	
ice thickness control failure	4
improper operation of ice agitator	1

peak demand and building characteristic data than are currently available. Such data will be of value to architects, engineers, and energy planners.

PLANNED ACTIVITIES FOR FY 1988

During FY 1988 we will continue to collect submetered data on the actual performance of installed systems from utility monitoring programs now underway. Our analysis will consist of comparing the cool storage system performance with estimated performance for conventional systems, as well as comparing the performance among the numerous buildings.

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Strategies for Reducing Urban Summer Heat Islands*

H. Akbari, J. Huang, and A. Rosenfeld

Urban climatologists and energy researchers have demonstrated that developed urban areas create summer "heat islands" with a typical daily average intensity of 3–5°C. In high-latitude cities with cooler weather, heat islands can be an asset in reducing heating loads, but in mid- and low-latitude cities, heat islands can contribute to the urban dweller's summer discomfort and significantly increase air conditioning loads. For example, the Los Angeles basin uses 5 gigawatts of air conditioning, an amount which represents $10 billion in power plants and another $5–10 billion for HVAC equipment. Ironically, much of this need for cooling energy is due to the man-made heat island brought on by urbanization.

The urban heat island results from the interaction of many factors, such as increases in the surface roughness and anthropogenic heat release from buildings and vehicles, coupled with decreases in the urban albedo and decreases in the evaporation rate which follow as trees and vegetation are replaced by impervious building materials. While some planners have regarded urban heat islands as inevitable products of urbanization, others have speculated that they could be alleviated by adding vegetative cover, spraying water on building tops, increasing the number of fountains and pools, choosing light colors for building exteriors, avoiding the use of dark-colored asphalt and bitumen in streets, altering urban dimensions, or minimizing the anthropogenic heat release rate.[1]

The objective of the heat island research at Lawrence Berkeley Laboratory is to *quantify* the energy saving potentials of such urban conservation strategies by developing and applying analytical models to simulate urban microclimates and the cooling energy requirements for buildings located within them. The results can be used to identify the most cost-effective methods for mitigating the urban heat island and to develop guidelines and suggestions for city planners, landscape architects, and architects. We have developed preliminary numerical models to simulate the effects on urban microclimates from changes in the amount of urban vegetation and the magnitude of urban albedo. Assuming that the changes are implemented city-wide, these models predict significant energy savings.

We have also begun addressing the constraints and possible conflicts that may arise in the implementation of such city-wide energy conservation measures. For example, if the number of trees and other forms of urban vegetation is significantly increased, the vegetation may block views, shade buildings excessively, and cause physical damage to urban structures through their branch and root systems. Similarly, increasing the urban albedo by using light colored paints and building materials may cause glare and increase construction costs. In gen-

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings Energy Research and Development, Building Systems Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

eral, the cost of poorly planned schemes to reduce the urban heat island could greatly reduce the benefits derived.

ACCOMPLISHMENTS DURING FY 1987

We have simulated the effect of increased vegetation on summer cooling loads of a prototypical house in four representative cities: Sacramento, Phoenix, Lake Charles, and Los Angeles.[2] The results are summarized in Table 1. Table 1 shows that the combined effects of shading and evapotranspiration on energy consumption is greatest in Sacramento, and lowest in Los Angeles. This is due to the difference in cooling hours between the two locations. The effect on peak power and cooling hours is greatest in Los Angeles, and smallest in Phoenix. This is again due to the fact that in Los Angeles, there are only 65 cooling hours per year, whereas in Phoenix, there are 3647 hours. The table shows that peak power savings on the order of 18%–30% is feasible.

In a separate study,[3] we have simulated both the direct and indirect effects of albedo changes on building cooling energy use in Sacramento during the peak summer period from July 9 to July 12. Results are presented in Table 2. Table 2 shows that a typical house with an albedo of 90% in a surrounding with an overall albedo of 40% consumes 62% less energy, has a 35% lower peak power demand, and experiences 44% fewer cooling hours.

Implementing the strategies we have discussed involves changing the urban environment in ways which will affect both public and private property. For instance, planting trees would result in conflicts such as who should pay for trees and what would be the effect of trees on the water supply. Similarly for albedo modification, the conflicts include the overall urban glare, choice of color, and who should be paying for urban modifications. In order to avoid conflicts, it is important that researchers and planners begin to integrate these strategies with all aspects of urban living. In many instances, public support and involvement will be essential. In reference to such

Table 1. Savings in annual cooling energy use and peak cooling power with increased urban tree canopy for the prototype house. All savings are with respect to the basecase described in the first column.

	Base-case	Savings from 10% increase (=1 tree/house)		Savings from 25% increase (=3 trees/house)	
Location		Shade Only (%Δ)	Shade+ evapotrans. (%Δ)	shade only (%Δ)	shade+ evapotrans. (%Δ)
Sacramento					
Annual kWh	1420	9	24	16	53
Peak kW	7.10	9	18	11	34
Cooling hrs	904	4	18	7	57
Phoenix					
Annual kWh	6911	3	13	6	33
Peak kW	8.87	5	9	6	18
Cooling hrs	3647	0.5	4	2	17
Lake Charles					
Annual kWh	3908	2	12	4	35
Peak kW	7.17	5	12	6	22
Cooling hrs	2489	1	7	2	24
Los Angeles					
Annual kWh	359	~ 0	~ 0	~ 0	~ 0
Peak kW	4.46	10	20	12	44
Cooling hrs	65	18	66	28	85

Table 2. Direct and indirect savings in cooling power and energy resulting from albedo modifications for the prototype house from July 9 through July 12. For cases where energy use increased, the numbers are given in parentheses. The albedo of the surroundings and of the house are represented as α_s and α_h, respectively.

Conditions					
House (α_h)	0.30	0.12	0.90	0.12	0.90
Surrounding (α_s)	0.25	0.25	0.25	0.10	0.40
	Basecase	Direct Savings		Direct + Indirect Savings	
		(Δ%)	(Δ%)	(Δ%)	(Δ%)
Energy kWh	74	(7)	19	(66)	62
Peak kW	7.07	(5)	14	(14)	35
Cooling hours	43	(2)	7	(37)	44

instances, we have studied[4] the importance of problem perception and have made clear that planners and resource managers cannot fully anticipate public attitudes and desires without enlisting the direct involvement of community members.

PLANNED ACTIVITIES FOR FY 1988

We have planned three major activities for FY 1988. 1) We will comprehensively study the windshielding and shading effects of trees in several representative heating and cooling climates in order to simulate the overall saving potential of trees. 2) We will organize a workshop among the heat island specialists, urban designers, and governmental offices in order to facilitate exchange of information among researchers. 3) We will continue our efforts to enhance our simulation capabilities such that we will be able to simultaneously simulate many aspects of the suggested mitigation measures.

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Analysis of Whole-Building Short-Interval Electric Load Data*

H. Akbari, K. Heinemeier, P. LeConiac, and D. Flora

As part of a statewide program, California utilities have collected 15-minute interval load research data for commercial buildings with time-of-use rate schedules and a connected load exceeding 500 kW. Some utilities have also conducted energy audits of commercial buildings as part of a survey of California's building stock. These databases provide valuable sources of *measured* information for analysis of energy use in California commercial buildings.†

The building characteristics, occupancy, and actual operation combine to create a unique demand "signature" in the building's load shapes. Some quantitative insights can be extracted from the 15-minute load data through a series of detailed analyses of temperature response, annual load-shape, frequency of equipment use, and comparisons of building load profile on the building's peak day with its profile on the utility's peak day.[1,2] While these analyses are by no means exhaustive, they form a basis for understanding the individual end uses of energy in commercial buildings without specifically monitoring them.

ACCOMPLISHMENTS DURING FY 1987

We analyzed load data and audits from eleven utility load research buildings. These buildings include four schools, three department stores, one refrigerated warehouse, three office buildings, and two hospitals, all located in Southern California. The data for these buildings contained 15-minute whole building, electric energy use data (kWh) for one year.

Many of our findings are used in a subsequent study to develop an algorithm for disaggregating whole-building load into its major end uses. The algorithm relies mostly on measured whole-building load for operating schedules of buildings and their HVAC systems. Our analysis has concluded that:

- Load research data are an invaluable source of information for analyzing and understanding patterns of customer electricity use, segregated by major end uses. Used to advantage, these data would provide a reliable basis for understanding and developing estimates of major end-use load profiles, by customer class.
- Buildings of the same category generally have the same characteristic load profiles, and, in many cases, the yearly load characteristics among the buildings of the same type are so similar that we can predict the building type merely by examining the load data.
- None of the buildings' annual peaks occurred on the system peak day in 1984. However, for all the buildings except schools, the load profiles on the system and building peak days are very similar.
- Analysis of the frequency distribution of hourly loads has yielded the expected values and variation of the hourly electricity consumption. An example of the frequency distribution of energy consumption during a shoulder hour is shown in Figure 1. Two distinct groupings are observed: one indicating normal operation of the building at that hour and one indicating early startup of the HVAC systems.

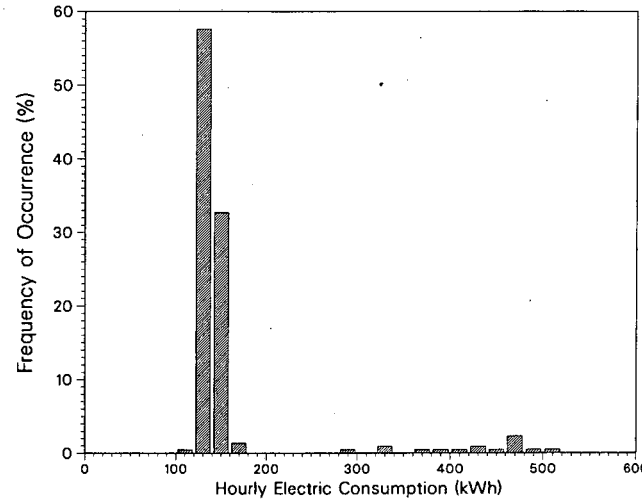

Figure 1. Frequency distribution of hourly load for an office building. Information about the building operation can be obtained by studying the distribution of the load across the year for each hour. Two modes of operations are indicated for the 7 a.m. shoulder hour. (XBL 8711-4707)

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings Energy Research and Development, Building Systems Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

†Although the data used in this study have come from buildings in California, the methodology and results can be applied to many commercial buildings having comparable load data.

- Hour-to-hour load variations provide information on seasonal changes in the operating schedules of a building.
- There is significant correlation between whole-building load and outside temperature for those hours that a building is air conditioned. This analysis has provided further information on the actual operating schedules of air-conditioning systems.

PLANNED ACTIVITIES FOR FY 1988

For FY 1988, we are planning to develop an integrated method to estimate commercial load shape and energy use intensity. The planned activity will build upon our analysis of the measured whole building load. One technique, which has already been tested on several buildings,[3] will exploit in-place energy management and control (EMCs) systems to obtain the whole-building data. We will also refine and apply our end-use disaggregation algorithm to estimate load shape and energy use intensities.

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ENERGY CONSERVATION POLICY

Overview

The Energy Conservation Policy Group continues to work in three general areas: research on energy conservation policies for commercial buildings in Southeast Asia, analysis of impacts of appliance efficiency standards in the United States, and assessment of impacts of demand-side programs on electric utilities, their ratepayers, and society.

The accompanying articles describe the main findings of the research and analysis in these three areas. Here we describe each of these efforts more generally, highlighting issues that are likely to be important in coming years.

The project on energy conservation in commercial buildings in Southeast Asia raises issues for both the United States and the developing world. Early research has shown the potential for significant energy and dollar savings in Southeast Asian buildings. Of the 12 billion spent annually on electricity for space conditioning, ventilation, and lighting in buildings in the five target countries (Indonesia, Malaysia, Philippines, Singapore, and Thailand), near-term savings of 10% ($200 million per year) can be achieved at relatively low investment and intermediate-term savings of 20 to 30% are possible, but with higher investment. A number of key technical issues need to be studied in much greater depth to know how best to achieve these savings. Knowledge is particularly weak on the performance of actual buildings in the region, methods for designing for natural ventilation, and procedures for achieving comfort (air conditioning and natural ventilation) at high efficiency. At the same time, a great deal is now known about increased energy efficiency in hot, humid climates through efficient lighting, improved window systems, better building envelopes, and daylighting of buildings.

The crucial question is how can government policy and private investment be translated into efficiency improvements in real-world buildings? The benefits—lower costs to the consumer, reduced oil use (the main fuel for electricity), and reduced drain on limited public capital for expanding electric power—are clear but the means to achieve these benefits is not so evident.

The project is now moving into a phase in which much more will be learned about these issues. A model conservation code for the region has been prepared. An in-depth analysis of the impact of a similar code in one country has been initiated. Now work is beginning on formulating broader policy approaches and increasing private sector involvement in energy conservation investments. The next several years will undoubtedly lead to much greater understanding of some factors that can stimulate and others that will retard effective policy implementation in a vibrant group of developing nations.

The appliance standards effort, while focused on the United States rather than the developing world, raises similar issues. The project has learned a great deal about the availability and costs of options to increase energy efficiency of residential appliances. It has also gained considerable knowledge about efficiency choices by consumers through its effort to forecast efficiency in the absence of standards. More recently, a model of the impacts of higher efficiency products on appliance manufacturers has been developed and applied. All of this work taken together appears to demonstrate that the market, if left to its own devices, will underinvest in energy efficiency by a significant amount. Findings from the analysis of manufacturer impacts show that an individual manufacturer is likely to lose money if it greatly increases the efficiency of its product offerings (everything else remaining unchanged and the efficiency increase cost-effective). However, if all manufacturers increase efficiency at the same time (as under standards), profits are much more likely to remain unchanged or to increase rather than to decline. In short, the analysis of appliance standards suggests that active policies are required if the benefits of higher efficiency appliances are to be achieved.

The utility analysis confronts similar themes—relating to the adoption of socially beneficial energy efficiency measures—but in the context of a regulated electric utility, its regulators, and its customers. Here again the basic issue is: what is needed to spur cost-effective investment in energy efficiency and other demand-side measures? It is probably too early in the research effort to draw conclusions. However, because the project is now working closely with electric utilities (directly and through utility organizations) and with their regulators (directly and through the National Association of Regulatory Utility Commissioners), insight into this issue is likely to emerge in the coming years.

In short, a major theme of the Energy Conservation Policy Group involves the complex interaction among many different groups in the process of studying, formulating, refining, and (in many cases) ultimately adopting and implementing policies to improve the efficiency of energy use in a cost-effective way.

Energy Conservation Policy for Commercial Buildings in Southeast Asia*

M.D. Levine, H. Akbari, J. Busch, S. Byrne, J.J. Deringer, K.H. Olson, I. Turiel, and M. Warren

The overall purpose of this project is to stimulate the development and implementation of policies to increase the efficiency of energy use in commercial buildings in five countries in the Association of South East Asian Nations (ASEAN): (1) Indonesia, (2) Malaysia, (3) Philippines, (4) Singapore, and (5) Thailand. This is carried out through training, research projects, analysis and assessment, and information dissemination.

Previous research demonstrated that significant energy savings in commercial buildings are possible. Figure 1 shows the types of measures that can reduce energy costs and the magnitude of savings that can be achieved. This figure makes clear that the largest reductions in energy use are for windows and lighting measures and that the overall reductions are substantial (more than 20% for daylighting alone). These large savings are particularly impressive when one recognizes that Singapore, for which the analysis was performed, already has among the most energy efficient buildings of any place in the tropics, having instituted an energy conservation standard in 1979 and having now achieved full compliance with the standard. For the ASEAN region as a whole, 20% savings (achievable in a ten-year time frame with a payback of two to four years) represents an *annual* electricity savings of about $400 million. (More than one-third of the electricity used in the region is in commercial buildings.)

*This work was supported by the U.S. Agency for International Development through the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

ACCOMPLISHMENTS DURING FY 1987

There were three different training activities during FY 1987: (1) courses in energy auditing of commercial buildings, with each course having 20–30 participants, conducted in Indonesia (twice), Thailand, and Malaysia, (2) a week-long workshop in Singapore for ten ASEAN delegates, covering research and policy activities of the project, and (3) a training course for four ASEAN delegates at LBL dealing with research on natural ventilation. In addition, the project supported ASEAN participation in a major conference in Singapore of the American Society of Heating, Refrigeration, and Air-Conditioning Engineers (ASHRAE) and attendance at other meetings and workshops throughout the region.

Research conducted at LBL included completion of wind tunnel work on natural ventilation in buildings, emphasizing effects of the external environment and interior partitions; completion of a users' guide for modeling natural ventilation in buildings; and parametric studies using DOE-2 on measures to increase efficiency of air conditioning use. The most important aspect of the research effort was the design

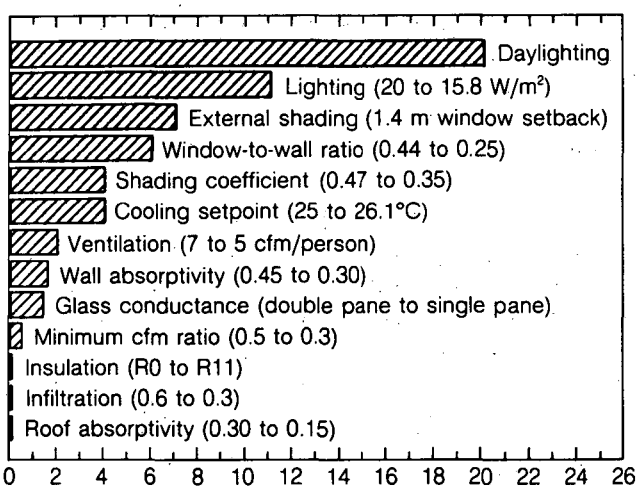

Figure 1. Reduction in total energy use (%). (XBL 841-68A)

and setting up of research projects within each of the ASEAN countries. A total of 26 research projects were initiated. These involved studies of such topics as energy auditing and monitoring of commercial buildings, preparation of natural ventilation design guides, assessment of the performance of energy management systems in buildings, computer simulation studies of the energy performance of buildings, and the analysis of policies to increase the energy efficiency of buildings in ASEAN.

In the area of assessment and policy, three documents of considerable importance to the overall project were completed.[1-3] The first is a model code for energy conservation in new commercial buildings. This is an innovative, detailed document that will provide the basis for standards and guidelines, as well as other policies, for the ASEAN region. The second document is an analysis of the energy and economic impacts of standards in one country. This will provide a basis for ASEAN researchers to evaluate their own policy approaches. The third document is a survey instrument to be employed throughout ASEAN to obtain data about extra energy use in buildings and decision-making on energy efficiency.

In short, the project has accomplished many of the key activities needed to set the stage for policy formulation on energy conservation in commercial buildings in ASEAN.

PLANNED ACTIVITIES FOR FY 1988

The project is expected to emphasize the following areas in FY 1988: (1) technical support from LBL for the research projects located in the ASEAN region, (2) continued training and workshops in selected areas of research and analysis, (3) engagement in a dialogue with public and private sector participants in ASEAN on policy development (using results of the project), (4) broadening policy research to include energy pricing reform and other economic policy vehicles to achieve project objectives, and (5) expanding the role of private sector participants and technology transfer in the project.

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Analysis of Federal Appliance Efficiency Standards*

H. Ruderman, P. Chan, P. Cunliffe, A. Heydari, J. Koomey, M.D.Levine, J.E. McMahon, T. Springer, S. Stoft, I. Turiel, and D. Wood

LBL is responsible for an integrated analysis of the impacts of federal appliance efficiency standards. The research involves a detailed assessment of the impacts on consumers, manufacturers, electric utilities, and on the nation as a whole. Our analysis is carried out in four major tasks: (1) an Engineering Analysis to quantify the efficiency improvements of various design options and their costs; (2) a Consumer Analysis to project the energy use, shipments, purchase price, and operating costs of more efficient products; (3) a Manufacturer Analysis to determine impacts on the appliance manufacturing industry; and (4) an Impact Analysis to examine the impacts of standards on various groups. The latter includes changes in consumer life-cycle costs, competition within the manufacturing industry, fuel savings and reduced need for new generating capacity by electric utilities, an assessment of environmental impacts, energy savings by fuel type, and the net present benefit of standards to the nation. Figure 1 shows how the parts of the analysis are interrelated, and how they fulfill the legislative requirements for evaluating the impacts of standards.

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings Energy Research and Development, Building Systems Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

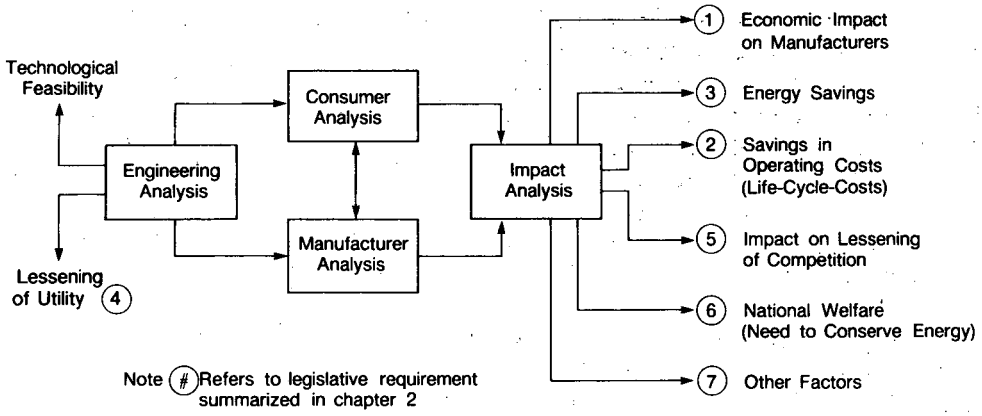

Figure 1. Satisfaction of legislative requirements through the analysis process. (XBL 856-8918)

ACCOMPLISHMENTS DURING FY 1987

In March 1987, Congress passed and the President signed the National Appliance Energy Conservation Act (NAECA)[1] establishing efficiency standards for household appliances. The legislation provided for periodic update of the standards by the Department of Energy. The first update will be for refrigerators and freezers, which DOE plans to complete by the end of 1988. DOE is also required to set standards for small gas furnaces (<45,000 Btu/h input) and to consider setting standards on television sets. Work during FY 1987 focused on analyzing the impacts of the NAECA and on supporting DOE's rulemaking on refrigerators, freezers, small gas furnaces and television sets.

Analysis of the NAECA Standards

NAECA prescribes energy performance standards for major energy-using household appliances and space conditioning equipment. Several improvements were made to existing data and models for our analysis of these standards. We incorporated a new method using discount rates and lag factors in the forecasting model to predict appliance efficiencies in the absence of standards. The manufacturer impact model was used to estimate the effects of standards on heat pump and central air conditioner manufacturers. Conclusions from this analysis were applied to other parts of the industry. We also developed methods for evaluating impacts on electric utilities and the environment.

Our analysis shows that in general the impacts of the legislation on consumers, appliance manufacturers, electric utilities and the nation as a whole are beneficial. The standards are estimated to reduce residential energy consumption by 16 Quadrillion Btu (Quads) during the period 1990 to 2015. Figure 2 shows that the annual savings grow to 0.95 Quads by 2015. More than 90 percent of the reduction is in electricity use. The largest energy savings are achieved for refrigerators, followed by water heaters and central air conditioners. These savings are shown in Figure 3, along with the net present benefits of the standards. Because most of the electricity saved at the margin is generated from gas and oil, about 60 percent of the energy saved is likely to be in the form of gas and oil and the remainder in the form of coal, nuclear, and hydroelectricity. The standards are estimated to eliminate the need for 16,000 MW of new generating capacity by 2015, mostly in peaking units.

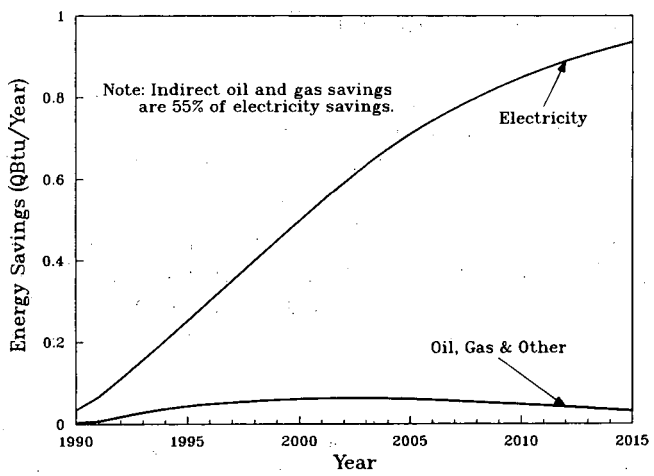

Figure 2. Annual energy savings of NAECA standards. (XCG 8711-11474)

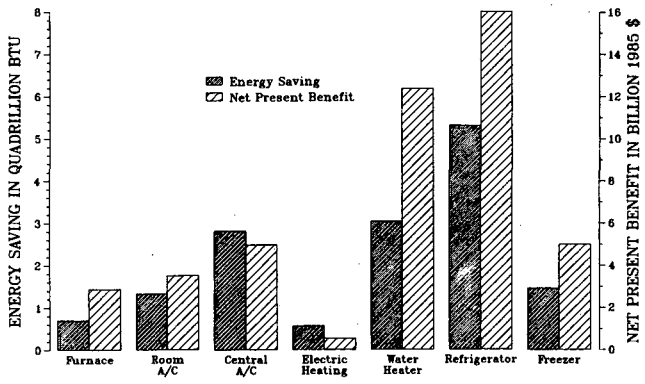

Figure 3. Energy saving and net present benefit of NAECA standards by product. (XCG 8711-11475)

The impact of the standards on consumers appear to be favorable for nearly all classes of products based on a decrease in life-cycle cost ranging up to several hundred dollars per new appliance. The net social benefit of the standards (evaluated at a social discount rate of five percent) is about $35 billion using average energy prices and $48 billion using one set of estimates of marginal electricity costs. The impacts on the appliance manufacturing industries as a whole are found to be negligible. However, the small high-cost segments of some industries (never more than 10 percent of an industry) may suffer a loss in profit of up to one third. The environmental impacts of the legislation appear to be favorable, particularly in reductions of emissions from electricity generation. However, the standards could increase chlorofluorocarbon production by about one percent, possibly leading to adverse health effects due to increased exposure to ultraviolet radiation. We have documented our analysis in a draft LBL report,[2] which will be submitted for publication.

Refrigerators, Freezers, Small Gas Furnaces, and Television Sets

The Engineering Analysis collected and compiled data on the efficiency and cost of designs options for the products being considered for standards. Much of the data collection was performed by subcontractors and consultants who are familiar with the industry. LBL staff visited several appliance manufacturing plants to obtain data and discuss energy-efficient designs. We adapted the ADL Refrigerator/Freezer Model to analyze the energy performance of refrigerators and freezers incorporating these designs. Input data for the model were obtained from appliance manufacturers and suppliers of components. Data collection for other products has been completed by the subcontractors, and their final report will be ready in the first quarter of FY 1988.

A major part of the effort during the year was in modifying and updating the LBL Residential Energy Model (REM) used to forecast appliance efficiency, shipments, prices, and energy use. A new method for forecasting completions by house type and state was incorporated in the model. The model now can calculate the number of households that are potential purchasers of small gas furnaces. New cost-efficiency data from the Engineering Analysis were added, and the algorithm for forecasting efficiency changes with and without standards was improved. We derived market share elasticities for small gas furnaces. More details of the changes made to the LBL-REM may be found in the accompanying article by McMahon and Chan.

The Manufacturer Analysis concentrated on rewriting the Typical Year Model (LBL-TYM) for use in the current analysis. From industry financial and economic data, the model estimates the market power of a typical firm, and from this estimate and the assumption that firms maximize profits, it computes a markup. The markup then determines the extent to which the firm can pass through its costs to consumers. The spreadsheet model is convenient for displaying and changing financial parameters, and it presents a balance sheet for the firm in an easily understood format. It also provides a Monte Carlo facility which makes a large number of runs with inputs chosen randomly to reflect their uncertainty. During these runs the output is automatically saved and analyzed; this reveals the uncertainty in the model predictions. We met with a panel of experts on the refrigerator and freezer industry and the gas furnaces industry to present the model and obtain data on the financial parameters.

The Impact Analysis methodology will change little from that used for the NAECA standards. Some issues in calculating marginal electricity costs and using them in calculating net social benefits have been resolved with DOE. We are fully documenting our analysis in a Technical Support Document (TSD) that will be published by DOE in conjunction with their Notice of Proposed Rulemaking (NOPR) regarding the first update to standards.

PLANNED ACTIVITIES FOR FY 1988

The analysis of standards on refrigerators, freezers, small gas furnaces and television sets will be completed in the first quarter of FY 1988. A draft of the Technical Support Document will be submitted to DOE at the same time. DOE will publish the

TSD and the NOPR in the spring of 1988. Additional analysis of these products may be required during FY 1988 depending on the comments received on the two documents. DOE is expected to issue the final rule in January 1989.

We will also analyze the impacts of possible amendments to the standards on clothes washers, clothes dryers, and dishwashers during FY 1988. Engineering data on design options have already been collected. We anticipate little change in the analytic methodology. Toward the end of FY 1988, we will begin examining new data sources and possible model improvements for the future analyses mandated by NAECA.

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The LBL Residential Energy Model*

J.E. McMahon and P. Chan

Detailed forecasting models have been used since the mid-1970's to assess potential impacts on consumers of proposed federal energy conservation policies. The first such model intended as a policy analysis tool for the residential sector was the Oak Ridge National Laboratory (ORNL) Engineering-Economic Model of Residential Energy Use.[1] A version of the ORNL Model was moved to LBL and adapted for an analysis of Consumer Product Efficiency Standards in 1979 (see Fig. 1). Public comments during the rulemaking process and new analyses at LBL have suggested many changes in the methodology for simulating residential energy consumption. Some of those changes have been implemented and described in U.S. Department of Energy publications,[2,3] conference proceedings, LBL reports, and previous LBL annual reports describing the analysis of mandatory appliance efficiency standards.

The accumulation of major changes to the method, including a new analysis of fuel and technology choice for space heating and cooling in new buildings, makes the LBL version of the ORNL model unique. The increasing availability of data and the need to analyze issues raised by interested parties in the rulemaking process have driven the transition from the ORNL to the LBL Model. The major methodological differences include: representation of recent equipment efficiency trends, forecasting of future appliance efficiencies based on an analysis of market behavior during the last decade; calculation of appliance replacements based on historical purchases and retirements; the data base for equipment costs and efficiencies; and treatment of competitive space conditioning systems (including heat pumps and small-capacity gas furnaces). In addition, the LBL Model has been integrated with

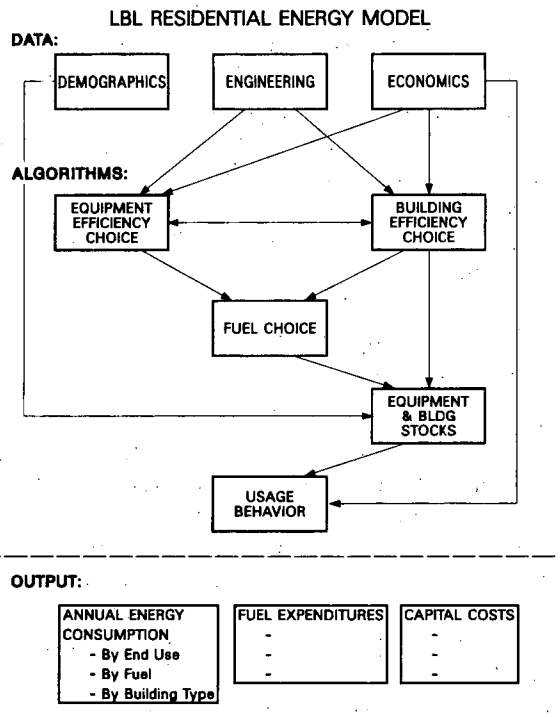

Figure 1. Logic diagram showing major components of LBL Residential Energy Model. (XCG 8412-13510)

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings Energy Research and Development, Building Equipment Division of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.

other tools for the study of individual electric utilities. A recent description of the current model, including changes to the original ORNL Model, is available.[4]

ACCOMPLISHMENTS DURING FY 1987

The space conditioning market share elasticities have been replaced.[5] The new method draws on the household-specific data from Annual Housing Surveys (1975–79), the same data used by REEPS (the EPRI-sponsored residential end-use demand model). Furthermore, the new method gives elasticities that vary with the size of the perturbation in the independent variables; links room and central heating choice; and links central air conditioning choice to space heating choice. In addition, those housing units having small heatloads can be treated as a separate market segment when analyzing market choice of heating and cooling fuel and technology.

The *accuracy of previous forecasts* of equipment efficiency and shipments has been assessed.[6] For many products, the changes in method and data have improved the accuracy. Those areas with the largest remaining forecasting errors have been identified.

A version of the LBL Residential Energy Model has been developed for use on personal computers. This greatly increases the transportability of the model and makes it more accessible to a number of users.

Regional disaggregation of the model has been completed. The input data for ten Federal Regions has been gathered. All demographic inputs have been benchmarked to the 1980 Census.

Equipment prices have been reestimated to include different markups by market segment. This provides a better characterization of the real-world pricing structure, including the importance of the builder market.

The impacts of the National Appliance Energy Conservation Act have been analyzed, and are reported in an accompanying article.

PLANNED ACTIVITIES FOR FY 1988

New analyses will be performed of national consumer, energy, and market impacts of possible federal appliance efficiency standard levels. Appliances under consideration include: refrigerators, refrigerator-freezers, and freezers; small gas furnaces; televisions; clotheswashers; dishwashers; and clothesdryers.

Updated engineering and pricing information regarding alternative equipment designs will be incorporated into the data base as available.

The interaction between internal loads (e.g., waste heat from refrigerators) and space conditioning energy use will be incorporated in the LBL Residential Energy Model.

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Analyses of Energy Intensities and Load Shapes*

H. Ruderman, I. Turiel, J.H. Eto, and K.E. Heinemeier

The California Energy Commission (CEC) every two years prepares forecasts of electricity demand and peak loads in the state. Over the past ten years the CEC staff have developed a series of models and methods used to prepare these forecasts.[1] The CEC now wants to improve the data used in their forecasting models for the *1989 Electricity Report*. They have contracted with LBL through the U.C. University-Wide Energy Research Group to provide data on (1) commercial sector end use intensities and (2) residential end-use load shapes for use in their models. The two subprojects started during the summer of 1987 and will continue for one year.

End-use energy utilization intensities (EUIs) are needed for electricity demand forecasting and for conservation policy analysis. Various methods have been used to estimate commercial sector EUIs for the California utilities. Because end-use metering is very expensive, most EUI studies rely on some combination of survey data and statistical and engineering analyses. The resultant wide variation in EUI estimates for some end uses and building types tends to reduce confidence in the results. The first phase of this project will provide a detailed comparison of the definitions and analytical methods used to generate commercial EUIs, recommendations for resolving differences, and a list of topics requiring additional data collection or research. Where data are available, EUI estimates will be compared to actual metered data, and needs for further end-use monitoring identified. The second phase will consist of a pilot project with Southern California Edison (SCE), for which EUIs will be calculated using on-site survey data, 15-minute interval whole-building load research data, and the DOE-2 Building Simulation Model. Initially, the survey data will be analyzed to develop descriptions of representative building prototypes. DOE-2 will be used to estimate space conditioning energy used based on these descriptions. All estimates of EUIs will be reconciled to the measured load shape and billing data.

The California Energy Commission has developed and used peak load models to forecast electric load growth in the residential and commercial sectors. The models calculate hourly loads on peak days based on end-use specific daily load shapes, for both weather-sensitive and non-weather-sensitive end uses. The purpose of this part of the project is to analyze available metered data on end-use load shapes to refine the current estimates used in the CEC peak demand models. Initial emphasis will be placed on residential loads because of data availability; future work will concentrate on non-residential end uses. The 17 end-use load shapes currently in the CEC Residential Peak Load Model[1] will be compared to monitored data collected by California utilities and out-of-state sources. Where necessary, the existing load shapes will be modified or replaced by those derived from the more recent data. The project will also assist the Commission staff in laying the groundwork for transforming the peak demand models into models that forecast hourly loads throughout the year, based on LBL's experience in constructing and validating its Residential Hourly and Peak Load Model.[2]

ACCOMPLISHMENTS DURING FY 1987

Commercial Sector End-Use Energy Intensities

During the early part of this project, we gathered data and reports describing previous EUI studies carried out for California utilities. We received all of the reports and started analyzing the survey data tapes that were used in these analyses. We also obtained and began validating a more detailed on-site survey of data for 375 SCE commercial buildings.

Several meetings have been convened with SCE and CEC to coordinate this project with one that will develop end-use load shapes for the commercial sector. A detailed workplan is being developed to combine these two projects so that they use common data and arrive at one set of EUIs and load shapes.

Residential End-Use Load Shapes

During the first few months of the project, we focused on identifying sources of residential load shape data. Contacts were made with investigators doing load shape research in the major California utilities, out-of-state utilities, EPRI, and other research organizations. We began collecting and reviewing published reports containing residential end-use data. We obtained a copy of the CEC Residential Peak Load Model and reviewed the algorithms and input data requirements.

*This work was supported by the California Energy Commission through the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.

We convened a workshop on residential load shapes in September which was attended by 35 people representing the CEC, all five major California electric utilities, and selected consulting firms. Talks were given on how load shape data are used in the CEC and LBL models for forecasting and impact analysis. Several utilities described their residential monitoring programs. There were two talks on using statistical procedures to disaggregate whole house loads into end uses. Based on the workshop and our other contacts, we are preparing a report to CEC summarizing available end-use data.

PLANNED ACTIVITIES FOR FY 1988

Commercial Sector End-Use Energy Intensities

During the coming year, we plan to achieve two major objectives:

(1) Review all California EUI studies and attempt to reconcile differences in estimated EUIs by the use of common definitions of business types, floor area, etc.
(2) Develop estimated EUIs for the SCE commercial sector using on-site survey data and load research data from SCE.

When the first objective is accomplished, we will recommend a common set of definitions to be used in future EUI studies. The data developed in reaching the second objective will be utilized by both CEC and SCE in future electricity demand forecasts.

Residential End-Use Load Shapes

Activities for the remainder of the project will center on the collection and analysis of data on the weather-sensitive and non-sensitive residential end-use load data. We are planning to obtain the data from utilities in the form of hourly loads by end use for each house in the sample. We will ask for data that is cleaned and verified. Auxiliary information, such as hourly weather data and household characteristics, will also be collected. The analysis will aggregate the data over households and utilities where appropriate and over time periods to get daily load shapes for typical days. For the weather-sensitive end uses, we will construct the time-temperature matrices required by the CEC Peak Load Model. The data from different sources will be compared and combined to arrive at the final load profiles.

The results of our analysis will be presented to the CEC in the form of machine-readable files. We will also submit three interim reports on data sources, non-weather-sensitive load shapes, and weather-sensitive load shapes, as well as a final report documenting the entire project. The final report will also include recommendations for improving the CEC model.

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Least-Cost Planning for the Pacific Gas and Electric Company*

E. Kahn, C. Pignone, and G. A. Comnes

The goal of this project is to develop methods for evaluating demand-side programs explicitly within the context of the traditional electric utility resource planning process, an approach that is generally known nowadays as least-cost planning (LCP). The project is designed as a study of the Pacific Gas and Electric Company (PG&E) and is partially funded by the company. The analysis is based on the use of an Electric Power Research Institute integrated utility planning model, the Load Management Strategy Testing Model (LMSTM), for production costing and forecasting, the DOE-2.1 building energy simulation model, for demand-side effect estimation, the LBL Residential Energy Model (LBL-REM) for electrical load forecasts, and locally written software for program evaluation and cost benefit analysis.

Following the completion of the calibration of LMSTM to the detailed production costing models used at PG&E, a LCP exercise based on large-scale implementation of two demand-side programs was carried out through several time horizons. The first test case is a somewhat hypothetical one that estimates the consequences of widespread adoption of the emerging thermal energy storage (TES) technology in commercial buildings. The second program (RAC) draws on past LBL work and involves the implementation of an efficiency standard for new residential room air conditioners, central air conditioners, and heat pumps installed in the PG&E territory.

ACCOMPLISHMENTS DURING FY 1987

The two test cases were completed and they show diverse results and illuminate different methodological issues. The analysis of TES begins with an elementary estimation of market penetration, which in the absence of better information is the only approach possible. All results, therefore, rest on assumptions of customer acceptance, as is usually the case in demand-side analysis. The RAC case couples the sophisticated capabilities of LBL-REM to the policy screening capability of LMSTM. Using LBL-REM gives greater plausibility to estimates of energy and load effects but only at the expense of tricky consistency problems.

Interesting results were obtained for the two cases studied. TES is a winner for customers and society and the results suggest incentives are not needed to accelerate adoption of this emerging technology. The heavy demand charge in the current PG&E large customer rate schedule itself provides a sufficiently strong load shifting incentive.

The RAC case is driven by the high customer costs of efficient appliances and comes out a net loser from the societal and customer perspectives. But it is a winner to PG&E because the costs are borne by customers through appliance purchases whereas the costs of efficient appliances are borne by customers. At a time of capacity expansion, higher oil and gas prices, and, therefore, higher prices for purchase power, this program could be justified, but these conditions are not likely to exist for PG&E until the later years of this century, so timing of the program becomes a critical factor.

The LCP principle is simple, but implementing it is remarkably complex. The experience of this study suggests that comprehensive planning with today's tools and methods is a task beyond the reach of most utility planning departments. Using mainframe models requires the dedication of a significant staff and achieving LCP literacy is a lengthy process. Carrying out analyses requires constant compromises and approximations, that, in some cases, can drive results. Certainly, the chances of LCP being reduced to a routine process are slender and the search for the ultimate LCP model appears futile. Further, the concept of LCP rests on assumptions about the industry as a whole that are not likely to hold over time. Notably, the steady infiltration of competition into the industry is eroding the assumption of a vertically integrated monopolistic utility.

PLANNED ACTIVITIES FOR FY 1988

This project, as outlined, was essentially complete at the end of FY 1987. The remaining work involves documenting the work done and reporting to PG&E. The models and methods are now in place to carry out a full LCP exercise for any utility service territory for which adequate data and company cooperation is forthcoming.

*This work was supported by the Pacific Gas and Electric Company and the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings Energy Research and Development, Building Systems Division of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.

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INTERNATIONAL ENERGY STUDIES

Overview

The International Energy Studies (IES) Group has been involved in research on energy demand since 1979. The work of the IES Group focuses on two areas: (1) energy demand in the industrialized countries; and (2) energy demand in the developing countries. The research on industrialized countries primarily addresses energy use in buildings, though work on the power generation sector is also underway. The research on the developing countries looks at demand in all sectors and also examines issues of energy supply.

The guiding philosophy of the Group is that understanding the evolution of energy demand requires careful examination of the structural forces that shape demand for energy, as well as the economic parameters. We seek to relate changes in energy demand to changes in the physical setting for energy use, looking in particular at changes in the efficiency of each energy end-use. We use comparisons of different countries to establish a context for understanding the observed patterns and for assessing trends in energy consumption.

The IES Group, which consists of scientists of different disciplinary backgrounds, is international in composition and multi-lingual. Visiting researchers from many different countries have been and are active participants in IES projects. The Group's work is a major activity in the Energy Analysis Program at LBL.

ENERGY DEMAND IN DEVELOPING COUNTRIES

Since its beginnings in this area with a study of energy use and conservation in Kenya's modern economy, the IES Group has expanded its research into energy demand in developing countries in four continents. In work funded by the U.S. Department of Energy and by several major energy companies, we have examined trends in energy use and structural change in 20 major energy-consuming developing countries in Asia, Africa, Latin America, and the Middle East, which together account for about 80% of developing countries' energy consumption.

The goal of our work is to understand how energy demand has changed in response to (often) rapid economic growth and two oil shocks. We examine how changes in economic structure, energy-use efficiency, and fuel mix will change demands in the future. A particular focus is the extent to which the growing demand for oil in the oil-exporting developing countries would reduce the amount of oil exported. The reduced exports combined with the declining production of oil in the U.S. would increase reliance on oil from the Middle East.

In addition to research on energy demand, the Group has also been involved in a number of evaluations of energy supply options for particular developing countries. A new area of work is assisting the U.S. Agency for International Development in developing effective programs to encourage expanded deployment of economically viable renewable energy options, and to better manage the use of electricity in developing countries.

ENERGY DEMAND IN THE INDUSTRIALIZED COUNTRIES

The Group's research on energy demand in the industrialized countries provides consistent information on energy demand in many of the world's largest energy-consuming countries as well as a context to better understand changes in U.S. energy consumption. Beginning with a comparison between the U.S. and Sweden, the research has evolved to include 9 European countries as well as Japan, the U.S., and Canada.

We developed the first and only data base of residential energy use in industrialized countries, now used as a reference by the International Energy Agency, energy authorities in many countries, and major oil companies. We have published several overviews of industrialized countries' residential energy use, and separate studies of individual countries focusing on the reversibility of oil use and structural change in electricity demand.

Additionally, we have expanded the work to include the service and power generation sectors. Current work on the residential sector includes analysis of the evolution of gas demand in Europe, development of scenarios of future energy demand, and investigation into the impacts of lifestyle changes on future household energy use.

The Causes of Rising Transportation Oil Demand in the LDCs*

S. Meyers

LBL has been engaged in the analysis of energy use in the Less Developed Countries (LDCs) for several years. The LDCs have been the most important source of increase in world oil use since 1973, and the largest source of growth in LDC oil use has been the transportation sector. To better understand the dynamics of growth in this sector, it is necessary to look in detail at the structure of transportation in these major LDCs.

ACCOMPLISHMENTS DURING FY 1987

LBL gathered data on oil use, motor vehicles, and air travel for a number of LDCs.[1] For 15 major LDCs, combined oil use in transportation increased from 57 to 133 million tonnes oil equivalent (TOE) between 1970 and 1985. Transportation accounted for half of their total increase in oil use, and its share of total oil use rose from 46% to 49%. The growth in transportation occurred despite increase in the price of transportation fuels and substantial substitution (nearly 6 million TOE) of ethanol for gasoline in Brazil. For all LDCs (except China), the increase in gasoline use between 1976 and 1986 accounted for nearly all of the growth in total Non-Communist World gasoline consumption since 1976, and the LDC share grew from 12% to 17%.

Between 1970 and 1985, absolute growth in gasoline use was greatest in Mexico, Saudi Arabia, Venezuela, and Nigeria, all major oil producers with low domestic gasoline prices. Very high growth rates were recorded in Saudi Arabia (18% per year average), Nigeria (17%), and Taiwan (14%). For diesel fuel, the largest absolute growth was in Brazil, Mexico, and India. The fastest growth rates were in Taiwan (16%) and Nigeria (15%), but growth averaged 7% per year or higher for most of the 14 countries. For jet fuel, absolute growth was greatest in Saudi Arabia, Brazil, and Mexico, while the fastest growth rates were in Saudi Arabia, Nigeria, and South Korea.

Growth in Motor Vehicle Ownership

The main cause of the growth in oil demand has been increase in the number of motor vehicles in operation. The largest sources of growth in passenger cars have been Brazil, Mexico, Argentina, and Saudi Arabia. Brazil, Mexico, and Argentina have by far the most cars among LDCs. Ownership and growth in trucks is more evenly distributed among countries.

Across countries, car ownership increases steeply as gross domestic product (GDP) per capita rises. The increase is less strong for commercial vehicles. Car ownership relative to GDP per capita is high in Latin American countries with major auto manufacturing.

Since 1970, motor vehicle ownership has risen considerably faster than GDP in many LDCs, paralleling the experience of the low-income developed countries in the 1960. In Taiwan, for example, growth in passenger cars in the 1975–85 period was 3.3 times faster than growth in GDP, and growth in commercial vehicles was 2.2 times faster. In Japan between 1960 and 1970, similar values were 3.2 and 2.4. Taiwan's per capita GDP in 1975 was \$1700–\$1800, while Japan's in 1960 was about \$1700. In both cases, rising middle class income and the expansion of the motor vehicle production industry acted in a mutually supportive manner to bring rapid growth in motor vehicles.

Vehicle sales, and especially passenger car sales, are very sensitive to changes in GDP. In the major oil-exporting countries, sales rose rapidly after the oil price increases, but have fallen off sharply in 1986. The oil effect was less strong in Mexico and Venezuela, which already had relatively mature motor vehicle markets, than in Saudi Arabia, Nigeria, and Iran, where motor vehicle ownership was low prior to 1973. Vehicle sales also rose strongly in the rapidly industrializing countries. In Brazil, Taiwan, and South Korea, maturing of the motor vehicle production industry contributed to growth in demand caused by rising income. Sales in Brazil took off at a much lower level of GDP per capita than in Taiwan and Korea, where government policies have discouraged passenger car ownership (especially in Korea). In both cases, however (more so in Taiwan), sales of new motor vehicles have risen sharply in the 1980s. In the mostly-agricultural countries with large populations, motor vehicle ownership has risen modestly, but is still constrained by low income and government policies. In most of

*This work was supported by the Office of Policy, Planning and Analysis, the Assistant Secretary for International Affairs and Energy Emergencies, Office of International Energy Analysis, the Assistant Secretary for Fossil Energy, Office of Planning and Environment, and the Assistant Secretary for Conservation and Renewable Energy of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098; and by grants from British Petroleum Company, Chevron, Conoco Inc., Exxon, Shell Oil Co., Shell International Petroleum Co., Statoil and AGIP.

these countries, the market for commercial vehicles (particularly light trucks) has developed faster than for passenger cars.

Although rising income is the most important factor, growth in vehicle sales have been affected by other factors. Prices are relatively high in many countries due to taxation or lack of competition. Government policy affects vehicle supply and price by limiting domestic production or by placing restrictions or disincentives (high import duties and/or taxes) on imported and domestic cars. Domestic assemblers are often protected from external competition by import restrictions, but prices are high due to high taxation of imported components, taxes on completed vehicles, and in some cases, low production efficiency. In many countries, the domestic market is not large enough to support an efficient assembly industry, and too many assemblers competing for pieces of a small pie has led to inefficient use of capacity. Once the market grows past a certain point, as occurred in Latin America in the 1960s and in Taiwan in the late 1970s, economies of scale contribute to lower prices, which in turn helps the market grow.

The poor state of the road system in most LDCs and urban traffic congestion may have had some inhibiting effect on car purchase, but these factors probably affect usage much more than ownership. The same applies to fuel prices, though in countries where gasoline prices have historically been very high or very low they have probably had some effect on the passenger car market.

Growth in LDC Air Transportation

Between 1970 and 1985 the number of total air passenger-trips to and from and within LDCs increased 250%. Domestic travel within LDCs registered the highest growth, averaging 9.2% per year, while international travel between LDCs and international travel between LDCs and non-LDCs grew at 7.7% and 8.2% per year respectively.

Total passenger-km on LDC airlines in 1984 was about 10 times higher than in 1965. Three-fourths of the absolute growth took place after 1974. The fastest and most growth in air travel has occurred in Asia. There was steady growth in Latin America until the 1980s, when travel flattened out. There was no flattening out in Asia for either international or domestic travel. In Latin America, increase in international travel flattened out in the 1980s, but domestic travel was less affected. The highest absolute growth in passengers between 1976 and 1984 was in Saudi Arabia and Mexico, followed by India and Brazil. Nigeria, Saudi Arabia, Egypt, South Korea, Algeria, and Thailand all had growth in excess of 10% a year.

Across countries, air travel increases with GDP per capita, but some countries with similar GDP per capita have very different levels of per capita air travel. This illustrates the importance of country-specific factors in shaping demand for air travel. The correlation is stronger for domestic travel than for international. The ratio of growth between air travel and GDP varied considerably in the 1970-84 period, but was over two in most countries.

Factors other than income growth affecting LDC demand for air travel include the price and availability of flights and trip ground costs. For domestic air travel, physical and economic geography (diffusion of the industrial economy among cities) are important, as is the availability and attractiveness of alternative transport modes. For international air travel, influences include geographic location, the extent of international economic links, exchange rates and currency restrictions, cultural ties with nearby countries, and the number of citizens living abroad.

PLANNED ACTIVITIES FOR FY 1988

We will continue to investigate changes in transportation in major LDCs as part of the research activities of the International Energy Studies Group.

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Alternative Transportation Fuels: The International Experience*

J.A. Sathaye and B. Atkinson

Worldwide interest in alternative transportation fuels has risen considerably since the two oil price shocks in 1973 and 1979. The U.S. Department of Energy is studying potential alternative fuel programs for the U.S. transportation market. As part of this effort, LBL conducted an analysis of the international experience with alternative transport fuels and the implications for future U.S. activities.

ACCOMPLISHMENTS DURING FY 1987

LBL conducted an extensive review of existing worldwide alternative transport fuel programs during 1987. We concentrated on those programs which had achieved commercial development, or at least a significant pilot project stage. Detailed studies were done for Canada, New Zealand and Brazil.

Canada is of particular interest to the U.S. because of the similarity in the two countries between the transportation situation and the interdependence of their automobile industries. Canada began its programs in 1980, concentrating on natural gas as a source of liquified petroleum gas (LPG) and compressed natural gas (CNG). Programs focused first on LPG, achieving almost 2% of gasoline market penetration, and then on CNG, which achieved a smaller penetration. Government support played a key role in consumer acceptance of vehicle conversion and in industry construction of fueling stations.

New Zealand's programs demonstrate the benefits and costs of an ambitious energy independence program. New Zealand began its programs in 1979, aiming for greater energy self-sufficiency using its natural gas resources. A large investment was made in a synthetic gasoline plant, opened in 1985. This fuel now substitutes for 35% of the gasoline market. CNG substitutes for 10% of this market and LPG for another 3%. As in Canada, government incentives proved crucial to the startup and continuation of the programs. In the case of synthetic gasoline, investments were made based on an expected world oil price much higher than the prevailing price in 1987.

Brazil's alternative fuels programs offer the example of the most extensive effort made to displace oil in the transport sector. This country also based its commitment to a massive ethanol program on projected rising world oil prices. However, Brazil had the combined goal of reducing oil imports and reviving their sugar industry by using sugar cane as the primary alcohol feedstock. Unlike New Zealand, Brazil had a large domestic automobile industry, allowing a switch to alcohol vehicle production. Dedicated ethanol vehicles now comprise 90% of new car sales. The economic viability of Brazil's alcohol program has been debated since its inception, but the technical success and market penetration offer another example of the importance of government's role as well as the cooperation of key players.

In Europe, interest in methanol blends has risen considerably in the last decade. Part of the attention to alternative fuels derives from plans to phase out leaded gasoline by 1989. West Germany is the most advanced; a 3% methanol blend comprises nearly 80% of its gasoline market. There is some push for ethanol production from the countries with large agricultural surpluses. CNG is being used in Scandanavian countries with natural gas resources.

A number of developing countries possess large natural gas deposits and are implementing CNG programs. Pakistan, Thailand, Bangladesh, Argentina and Colombia are in the first phase of CNG use, and several others have pilot programs.

LPG has been used as a gasoline substitute in Europe since World War II, now meeting 11% of road transport demand in the Netherlands and almost 3% in Italy. LPG has penetrated certain markets in Japan, Korea, Thailand, Mexico and other countries, but its use in transport is not expected to increase because of its limited supply in the refinery petroleum product mix and competition from other uses.

Ethanol is used in transport in the Philippines and several African countries (Zimbabwe, Malawi, Kenya) for much the same reason as in Brazil: to bolster their sugar industries hit by low world prices. Both China and South Africa make methanol from coal.

The extent of further commercialization of alternative fuels is unclear due to the uncertainty of future oil prices. In countries such as New Zealand, government policies have shifted to encouraging the

*This work was supported by the Office of Policy, Planning and Analysis, the Assistant Secretary for International Affairs and Energy Emergencies, Office of International Energy Analysis, the Assistant Secretary for Fossil Energy, Office of Planning and Environment and the Assistant Secretary for Conservation and Renewable Energy, Office of Photovoltaics Technology of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098; and in part by grants from British Petroleum Company, Chevron, Conoco Inc., Exxon, Shell Oil Co., Shell International Petroleum Co., Statoil and AGIP.

private sector to take over the programs. In others, such as Argentina, lending agency support is critical. Brazil is considering ending subsidies for its alcohol program, and scaling down its new CNG/diesel substitution program to segmented urban markets.

Environmental and social impacts of alternative fuel programs were not a focus of our study. However, urban air quality has been an important motivation for several alternative fuel programs.

Lessons for the U.S. include the importance of government commitment and promotion, use of incentives such as guaranteed alternative fuel prices, grants and loans for conversion and fuel station construction, and fuel producer and distributor incentives. Information to boost public confidence in unfamiliar technologies is also essential. Involvement of state governments, automobile manufacturers, and energy companies in cooperation with the federal government is important in the initial stages as well as for the long-term economic success of alternative fuels. U.S. decisions on alternative fuel programs will influence those of other countries, particularly Canada, but also Europe and Japan, as well as the developing countries. Automobile manufacturers and conversion technology companies will be affected by the direction of U.S. programs.

PLANNED ACTIVITIES FOR FY 1988

A final report will be prepared, incorporating comments from reviewers from various countries. We will look more carefully at developments and prospects in Europe. Issues in alternative fuels programs include diesel substitution and the changing petroleum product mix resulting from reduced gasoline demand.

Renewable Energy Technologies in the Developing Countries: A Reassessment*

J. Sathaye and S. Meyers

Renewable energy projects in the developing countries have been supported by international lending and development agencies, by foreign assistance agencies in the industrialized countries, and by the developing countries themselves. The U.S. Agency for International Development (AID) has been involved in, or is currently supporting, over 200 programs which contain significant renewable energy components. Although there have been successful projects, the results have generally been much less promising than anticipated. The AID Office of Energy has been conducting a critical reassessment of AID's experience with renewable energy technologies. The reassessment is intended to clarify lessons learned and to help in setting future directions. LBL has assisted in this effort.

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ACCOMPLISHMENTS DURING FY 1987

In collaboration with other researchers, LBL reviewed many evaluations of renewable energy technology applications in the developing countries. While many projects have not proven successful over time, a number of technologies have been demonstrated to be reliable. Among these are small-scale applications of photovoltaic systems for communications and health clinics, small hydro for mechanical and electrical power, wind water pumping, some industrial-scale biomass fuel technologies, and improved charcoal stoves. Biogas, gasification, solar drying, and dendrothermal electricity have been difficult to apply successfully.

A lack of emphasis on involvement of the private sector for implementation and on commercialization was found to be a problem in many cases. Technologies that were not commercially proven were often problematic. A high degree of user involvement in project design and implementation was found to be an important ingredient for success. Participation in all phases of the project helps to ensure motivation and a transfer of technology. Many projects failed because they were not matched appropriately to local needs and social customs.

The availability and nature of local renewable energy resources, local human resources, and institutional capabilities are important to factor into design. Lack of attention to requirements for maintenance, spare parts, and local skills develop-

ment caused problems in many cases. Another difficulty for dissemination of renewables is widespread subsidization of electricity and diesel fuel.

In addition to assisting evaluation of renewable energy experience, LBL helped to organize a workshop that brought together individuals from the U.S. renewable energy industry and from AID-assisted countries, as well as AID staff and consultants.

PLANNED ACTIVITIES FOR FY 1988

LBL is assisting in the completion of a report on new directions for AID's renewable energy activities. This includes providing updated information on technology status and costs and evaluation of financing and environmental issues.

Electricity Utilities in the OECD: Energy Secure?*

D. Hawk and L. Schipper

During the 1970's, electric supply industries worldwide were confronted with a rapid succession of changes including oil supply disruptions and new government requirements to mitigate against environmental impact of energy use. The economic, technological, and political conditions under which electric utilities operated were in transition. Coming out of the 1970's, many utilities recognized the need to establish mechanisms (if not already in place) to anticipate change and respond to it in a controlled, constructive way, thereby maintaining the stability and/or security of electric supply.

ACCOMPLISHMENTS DURING FY 1987

In this work we investigate the ability of the electricity supply systems in five European countries — France, Germany, Italy, Sweden and the United Kingdom — to respond to changes in the accessibility of energy inputs or the operability of generation facilities.[1] Accessibility and operability could be determined by economic, political or technical conditions. We briefly describe what each system looked like in 1972–1973 and their immediate (short term) responses to the oil shock of 1973. We then explain how the systems have evolved since and in response to the shock, by default or through deliberate utility planning. In the short term how resilient would these systems be to a shock today? (Short term refers to the level of remedies that can be considered. In this case, additions to capacity cannot be considered).

What kind of responses are we looking for? Potential resilience could be indicated by three characteristics of the supply system. First, is the generation capacity in use based on a diverse mix of fuels, and if so, what are the load factors? Could the load factor of certain plants be increased in order to compensate for the loss in production due to the closing of other plants that use a fuel which makes them no longer reasonable to operate? The second characteristic is the share of the generation capacity which has dual or multiple fuel capabilities. Thus, if an event or situation precludes the continued reliance on one fuel, these plants can switch to generating with the second fuel. The third characteristic is the extent to which the country can import electric power from surrounding countries. Power imports are seen as supply options comparable to deciding which plants to generate from. However, this option is dependent on whether the supplying country can transfer enough power at the right time. In this analysis, we have not only considered the range of possible responses, which are largely derived from the technical characteristics of the system, but also any political or regulatory constraints that exist.

Although the first oil crisis put brakes on energy growth in most Organization for Economic Cooperation and Development (OECD) countries, electricity demand continued to grow, spurred in part by the relative decrease in electricity costs *vis a vis* those for oil. After the Iran crisis in 1979, electricity prices increased significantly in most countries. Some substitution of electricity for oil continued, but overall electricity growth rates were slower than before 1979, particularly in Europe. In OECD Europe, electricity as a share of total end use energy increased from 11.3% in 1973 to 16% in 1985. In conjunction with increased demand, the utilities' share of total pri-

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mary energy requirements in OECD Europe rose from 27.4% to 35.9% in the same period.

The reduction in oil use among Europe's electric utilities has in particular played an important role in the overall drop in OECD oil demand since 1973. In 1985, the five countries under study used 36.9 million tonnes oil equivalent (MTOE) in their 77 GW of oil-fired capacity. If these countries used their 1985 oil-fired capacity at 1973 load factors, 73.8 MTOE oil would have been used — twice the amount actually used! The 1986 drop in the price of oil made that fuel once again attractive to some utilities, raising additional concern that oil use in this sector might increase in the near future, particularly if lower oil prices lead to lower electricity prices and a further stimulation of demand. Thus, the backout of oil from the utility sector may not be permanent; indeed, oil use in the UK skyrocketed during a coal miners' strike in 1984. The utilities face the question "more oil, or less?"

The hazards of a heavy reliance on oil are all too familiar. As we contemplate the fuels which have been considered alternatives to oil, we find that they are now also suspect due to security and environmental problems. Natural gas, seen by many as the cleanest fuel, still has not penetrated significantly into the utilities sector in Europe, in part because of continuing concerns over security of supply. A large share of Europe's gas is imported from the USSR and Algeria.

The combustion of coal causes many severe environmental problems, including acid rain and the "greenhouse effect." In addition to the environmental and supply disruption that would be associated with "another Chernobyl", nuclear power poses significant environmental risks at the stages of fuel reprocessing and waste disposal. Many people are also concerned with the security of reprocessing facilities in the face of terrorist threats. Suddenly the utilities find themselves somewhat less sure of the alternatives to oil, and see their institutional footing challenged from many directions.

PLANNED ACTIVITIES FOR FY 1988

In FY 1988, the final section of this report will be completed. This section will synthesize, summarize, and compare the changes that have occurred in these five countries and discuss future expectations for electricity supply as expressed by utility management and government personnel.

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Energy Conservation Policies for Buildings in OECD Countries: Did They Succeed?*

D. Wilson, S. Tyler, A. Ketoff, and L. Schipper

Energy conservation policy seeks to improve the efficiency of energy use by speeding up market forces or correcting market failures. In this project, we identify energy conservation programs which have given positive results, and why, in countries outside of the U.S. To analyze the potential transfer of foreign experience to the U.S., it is essential that specific government policies and programs are considered within their national contexts.

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings and Community Systems, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

The project covers government conservation programs for the residential sector in Canada, Denmark, France, Japan, Sweden, United Kingdom, and West Germany.

ACCOMPLISHMENTS DURING FY 1987

Residential energy use dropped considerably in all Organization for Economic Cooperation and Development (OECD) countries after oil prices increased in 1973 and 1979. In some countries (Denmark, France), the drop has been abrupt, and was initially a consequence of behavioral response to price signals and information campaigns. In others (Canada, Sweden), progressive drops in consumption reflect the impact of conservation investments in the sector. An exploration of the factors determining the variation in household energy use allows an analysis of the impact of energy conservation policies in each of the countries studied.

We distinguish between a conservation policy, its programs, and individual packages of measures. The policy establishes the overall goals and justification; the program connects various government and private institutions to the energy user (or producer of energy systems), while the package is a group of individual measures that are physically implemented.

In Denmark, where the climate is severe (more than 3100 heating-degree-days (base 18°C) per year), the thermal condition of the building stock was poor in the 1970's. This fact, and the fact that comfort levels in Denmark were high, left room for substantial reductions in energy consumption in the residential sector. Survey data indicate that the Danish people responded to the energy crisis by rapidly modifying their energy consuming behavior. Later on, retrofits of the existing building stock played a role as incentive programs were refined and were eventually offered as a package under the "Act on the Reduction of Energy Consumption in Buildings" of 1981. This package included professional audits and after-the-fact inspections to ensure the quality of retrofit work performed, subsidies for an approved list of energy-conserving measures, and a home energy certificate system. A national mandatory building construction standard for new buildings was implemented. This standard is the most stringent in the European Community, and is second only to the Swedish building standard in the world. Prices and taxes are also key to residential energy policy in Denmark. In general, household energy prices are high in comparison to those of other countries. Residential energy taxes were increased once in December of 1985 and twice in 1986 in order to counter the effects of falling oil prices, thus keeping energy costs artificially high.

In France, the residential sector has played a key role in the government's energy conservation programs because of the large share of oil consumption attributed to this sector. Energy conservation program activity in this sector began in 1974 and emphasized information exhorting behavioral change and efficiency improvements with the early creation of financial incentives for investments via a system of tax deductions. Regulations for minimum levels of thermal insulation, appliance efficiency standards and strong emphasis on indoor temperature levels were also features of early French government intervention in this sector. Later in the seventies, grants tied to anticipated energy savings were introduced for the residential sector, but were terminated within a couple of years because of their high administrative costs, the difficulty of accurately determining energy savings in advance, and the small proportion of investment costs actually represented by the grant. Since the emergence of the AFME—the French Agency for Energy Management—in 1981, the program emphasis in the residential sector has been on providing decision aides to prompt effective private investment in energy efficiency, largely through subsidizing residential audits. An increasing effort has been made to assure home owners of the security of energy retrofit investments by emphasizing both the financial incentives (tax credits and low interest loans) as well as the technical competence of the work (through auditor training and savings guarantees). This emphasis supplemented the substantial capital investment by the Ministry of Urbanism and Housing, which was heavily involved in providing financial incentives for housing retrofits, particularly in the large public housing and co-operative housing sectors. In addition, through its regional offices, the AFME has become involved with several comprehensive local Pilot Community projects which have attempted to mobilize local agencies, contractors, financial resources, landlords, and housing occupants in community-based conservation programs.

In Japan, residential energy policy and the framework for conservation programs was articulated as a package in the "Law Concerning the Rationalization of Energy Use" of 1979. This Law was intended to address comprehensively the variety of areas in which energy savings could be made in the sector. Responsibility for carrying out the intent and requirements of the Law was placed upon The Ministry of International Trade and Industry (MITI). This had the dual effect of centralizing the development and implementation of energy conservation programs and of applying an industrial perspective to this key process. The latter limited the ability of the programs that grew out of the Law to capture a large part of the potential energy savings in the residential sector. Where industrial solutions could be applied, as in the case of appliance efficiencies, the Japanese programs excelled. Where energy waste fell out of industrial territory, as in the case of housing construction practices, MITI's impotence resulted in potential savings being left untouched: no mandatory standards for the construction of new buildings were developed and incentives for retrofitting existing housing stock were not offered.

West German residential energy policy is built on the premise that governmental intervention is appropriate only in those cases where market failures exist. The "Energy Conservation Act" of 1976 provides the framework and legal basis for policies and programs which were seen as necessary in order for

full and unhampered responses to market forces to take place. In 1978, the "Modernization and Energy Conservation Act" and the "Income Tax Act" provided a system under which grants and tax incentives could be used for encouraging the retrofit of existing homes in order to bring them up to the standard for new buildings. In addition to these standards and retrofit incentives, regulations for regular inspections and adjustments of heating equipment, individual heat metering in multi-family buildings, consumption-based billing practices, and appliance labeling were established. A "gentleman's agreement" for efficiency improvements was made with key actors in the home appliance industry. Despite the requirement for consumption-based billing, decreasing block rates are still in use for electricity, and part of the consumer's bill is based on the number of rooms in the dwelling (which is clearly divorced from actual energy usage). Because information programs in general disperse information upon request, at trade fairs, in magazines, and at local service centers, all of which require an initial action or "demand" on the part of the consumer, their effectiveness in providing information beyond that for which a market exists is questionable.

For each of these countries, we completed a broad evaluation of programs and policies which resulted in energy-saving activities that otherwise would not have been carried out. Very few detailed evaluations of conservation programs have been performed in the countries analyzed. Many of those which do exist have been completed by the same agencies responsible for the implementation of the programs. This might lead one to question the objectivity of the evaluations.

PLANNED ACTIVITIES FOR FY 1988

In FY 1988 we will complete the comparison of national energy conservation programs, and evaluate individual programs or packets of programs, focusing on how well those programs reached their intended participants, i.e., the consumers.

Energy Interdependence: Global Issues and Options*

L. Schipper, A. Ketoff, and J. Sathaye

An informal meeting was organized by members of the Lawrence Berkeley Laboratory's International Energy Studies Group in Berkeley, on May 30, 1987, to discuss a number of issues related to key aspects of the world energy system. Twenty-eight representatives of academia, government, and the private sector from the Americas, Europe, and Asia participated in the meeting.[1]

During the last two decades, the relative importance of the various countries and institutions on the world oil scene has changed; oil consumption in North America, Europe, and Japan is virtually unchanged from that of 1973, while in rest of the world it has continued to increase, reaching 43% of the world total in 1985, as compared with only 29% in 1970. Oil and energy *production* has also seen a restructuring. Finally, increased energy efficiency provided the greatest contribution towards reduced world oil demand; the impact of greater efficiency will continue to be felt even if oil prices remain low. In short, the energy system is significantly different from what it was in the early 1970s, yet many decisions are based on information and mental maps of the older system.

It is now clear that oil supply and its price, as well as efficiency of use, may be only one part of the story, one whose relative importance is diminishing. There are other concerns that in the long term may be more serious. Most notable is the worsening global environmental impacts of energy use. The time scale for global environmental change through man's intervention, spurred by energy use, is rapid in contrast with natural global climatic and environmental changes. The *ecological* and *political* time scales for responding to problems, once identified, are not well known. Unfortunately, the resilience of both human societies and the ecosystem to various energy-related "shocks" of varying rapidity, magnitude, and extent is insufficiently understood.

*This work was supported by Program Development Funds through the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

ACCOMPLISHMENTS DURING FY 1987

Concerns over the Energy System of the Late 1980's and Beyond

Among those topics that received the most attention on May 30 were the following:

- Global environmental disruption often has consequences not reversible on a short time-scale. The growing awareness of its link to energy production and use indicates that we may be approaching limits and critical decisions. Are present and future decision-makers prepared?
- A similar awareness of the links among energy, food, urbanization, and industrialization makes decision-making on the basis of energy alone both difficult and sometimes dangerous. How can present energy models and analysis paradigms be adopted into the wider human and economic context in which energy is but one variable?
- Accelerated restructuring of the demand for energy caused by changing economic growth patterns, rapidly evolving energy-use technologies, and even demographic forces has proven too complex to be handled by the data systems and models of yesterday. What can be done to improve our understanding of the system today?
- Increased energy efficiency contributed significantly to reduced energy and oil demand, relative to activity after 1973. Has the scope for improved efficiency narrowed, or will technology drive further improvements?
- Energy matters are now dispersed over a much wider circle of institutions, countries, and cultures than in 1973. What is the appropriate language today for understanding the problems and communicating the concerns in this diverse environment?
- The transformation of the world oil market into a commodities market with round-the-clock operation places a new actor between oil in the ground and the final consumer, namely the oil trader. How does this new layer of institutions affect the stability and long-term development of the world oil and energy market? What are the new *roles* of the actors, and the new *rules* under which they act?
- Availability and price stability of oil has been a major concern internationally. Does the current price of oil and increased availability mask impending shortages?
- The role of local biomass fuels (such as wood, charcoal, or dung, often termed "non-commercial energy") has been largely overlooked by national and international authorities, although this is the predominant energy form in many countries or regions. How would local, regional, and world energy decisions be affected if biomass and its associated problems are included in the picture?

These issues all point to the most important difference in the energy system of today *vis-a-vis* that of 15 years ago: the linkages between energy and other inputs and outputs in the economy, including human capital and information, have changed, and will continue to evolve with rapidly transforming dynamics of the world economy. The changing linkages could lead to future energy-related crises which would require adoption of new options important to both private and public institutions.

The consensus of the group that met in Berkeley was that a new approach is needed that will *quickly* sense global and regional changes in economies, geopolitical factors, and shifting demands for energy and its forms and sources. A new learning process could greatly improve our understanding of the linkages among energy, economic security, environment, and food. This process should be a new, international effort, far beyond that of a single study. Participation in such an effort would be open to experts from any country, and effort would be made to avoid groupings around familiar regional lines, i.e., North *vs.* South, industrialized *vs.* developing, etc. This effort could provide a forum to voice unencumbered views on controversial issues of international concern. As many of these links are too complex and are changing too rapidly for any single institution to follow, and are becoming more international and interdependent, only a decentralized effort could provide the forum for such an activity.

This forum will have as its primary responsibility the identification of issues and options, and the subsequent improvement of our learning and analytical tools to deal with them, in meeting the new kinds of energy-related problems we expect in the 1990's and beyond. Policy and economic analysis and synthesis from this effort will have an international perspective, which is essential to identify emerging global energy issues. An international perspective will provide a much more accurate determination of emerging perceptions and values regarding important energy issues. Policy development explorations will reflect interaction between experts from research institutions and policy officials from government and professionals from industry.

PLANNED ACTIVITIES FOR FY 1988

In FY 1988, the LBL group, with input from others joining the effort through computer networks, will carry out a new activity, provisionally called the Energy Roundtable Experiment. The Energy Roundtable will initially consist of several dozen energy decision-makers and experts from around the world. The Roundtable experiment will address itself to several of the issues outlined above through a series of position papers and electronic conferences. One or more individuals or groups will be asked to take the lead in developing each paper, but members of the Roundtable would be encouraged to contribute to each paper through the electronic medium, under the leadership of a motivator. The two topics chosen are energy and transportation in the future, and electricity in developing countries. Shell International Petroleum Company will make available an existing electronic conference channel through which this experiment will be carried out. If the experiment is successful, a larger effort will be launched later in FY 1988.

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RESOURCE MARKET MECHANISMS

Overview

The Resource Market Mechanisms group analyzes and conducts research on the methods used for the transfer of natural resources, particularly the transfer by means of formal competitive auctions from government to the private sector, as well as on broader energy policy issues.

The following article contains a description of an analysis of the design of auctions for the purchase by utilities of power from cogenerators and small power producers. In the past, we have studied auction design issues for coal leasing, timber sales, oil leasing, and the use of auctions by the State of California. There has also been modelling in support of natural gas deregulation policy analysis, and a study of U.S. energy vulnerability in the 1990's. We are currently interested in the use of auctions for deregulating all new electric power generation and in modeling the supply situation for alternate fuel vehicles.

Designing Auctions for the Purchase of Electric Power by Utilities under PURPA*

M.H. Rothkopf and E.P. Kahn

The Public Utilities Regulatory Act (PURPA) requires there to be procedures for electric utilities to buy electric power from qualifying cogenerators and small power producers (QFs) at rates up to "avoided cost". This has led to price-posting procedures at prices calculated as the utility's marginal cost. Unexpectedly large sales at these prices and slow adjustment to falling energy cost are partially responsible for payments to QFs in excess of the utility's true avoided cost. Using competitive bidding instead of posted prices has been proposed as a way to avoid this outcome.

ACCOMPLISHMENTS DURING FY 1987

We have written a report that reviews bidding theory and explores four issues that arise in designing auction systems for the purchase of power from QFs under PURPA.[1] (In addition, in one appendix it considers broader auctions involving non-QF bidders.) One of these four issues is the choice of auction format between progressive oral auctions, Dutch oral auctions, standard discriminatory or "first-price" sealed bidding (if you win, you get paid the amount of your bid), and nondiscriminatory or "second-price" sealed bidding (all winning bidders are paid the amount of the best losing bid). Another issue is the extent to which non-price factors influence the auction and the manner in which they do. A third issue is the way in which bid acceptance procedures deal with the discrete quantities of power offered by different bidders. For example, if a utility that needs 500 MW that it can supply at 10¢ per kWh receives three all-or-nothing bids, one offering 300 MW at 7¢, one offering 250 MW at 8¢ and one offering 200 MW at 9¢, which bids should it accept? The fourth issue is the frequency of auctions. After discussing these issues, the report explores practical details through a case study of a PURPA auction using publicly available data representative of conditions facing Southern California Edison Company.

With respect to auction format, the report recommends sealed procedures over oral ones. It identifies flaws in the arguments in favor of the economic efficiency of nondiscriminatory sealed bidding and recommends familiar discriminatory sealed bidding over the much less common nondiscriminatory format.

In discussing non-price features, the report notes the tradeoff between simplicity and economic precision. It identifies some factors, such as capacity value and transmission access costs, that are rela-

*This work was supported by the Director, Office of Policy, Planning and Analysis, U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.

tively amenable to differentiation into components with separate payment streams and performance factors. Others, such as financial risk (see Fig. 1) and dispatchability are not. It also notes with approval the approach taken in Massachusetts to deal with financial risk, and it notes the difficulty of dealing with dispatchability when it is important.

The discrete nature of bids can cause difficulties. There are many different ways to decide which of a given set of bids to accept. The report recommends that bid acceptance rules be spelled out precisely before an auction. The minimum cost selection of bids for meeting a given power requirement may involve accepting a bid with a higher unit cost than a bid that is rejected. It is undesirable for the utility to accept rigidly the discrete nature of the bids and select the set of bids that provides the desired amount of power at the minimum cost. The report recommends four measures that a utility can use to reduce the impact of the discrete nature of the bids. These are (1) encouraging multiple bids by a bidder offering incremental quantities, (2) allowing a marginal bidder to downsize the quantity offered if it is too big (given the other lower bids) to be acceptable, (3) allowing a reasonable tolerance in the definition of the required quantity, and (4) valuing excess power beyond the desired quantity at its value to the utility in deciding if a marginal bid is acceptable. With these four measures, the report recommends a bid acceptance procedure that considers bids sequentially in order of increasing cost per kWh. Such a procedure will have good economic and bidder incentive properties and will be more stable and "fairer" than a procedure that rigidly minimizes utility cost given the bids.

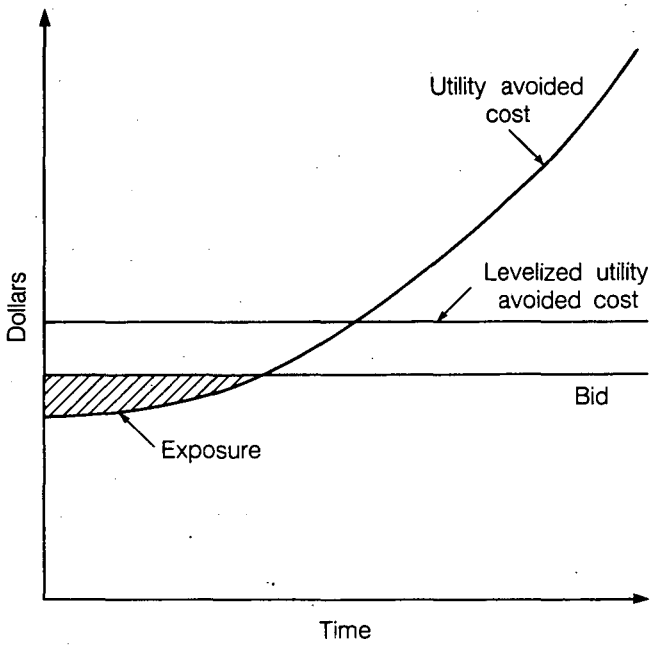

Figure 2. In an auction in which bidders bid both a price and a quantity, a bidder with a lower average cost curve (AC_10) and marginal cost curve (MC_1) can nonetheless be a high cost bidder if he estimates a higher price ($> P_1$) and selects the quantity to offer so that anticipated price equals marginal cost. (XBL 8711-4779)

The report recommends that PURPA power purchase auctions be held at least every few years if utility need for capacity allows and that they not be held at much shorter intervals. Too frequent auctions can put large projects at a disadvantage and facilitate collusion. Too infrequent auctions can put at a disadvantage time sensitive potentially attractive projects.

The Southern California Edison case study is based on cost conditions anticipated by the utility for the mid-1990's. It uses the UPLAN model to estimate avoided cost based on methods prescribed by the California Public Utilities Commission. We provide a simple characterization of the "demand curve" for power. Bidders are represented by cost functions approximating the opportunities available to natural gas-fired cogenerators in Southern California.

From the study, we have been able to observe that large-scale projects will cause difficulties in designing bid acceptance procedures, that estimation error can introduce some inefficiency in first price auctions, and that utility costs will exceed social cost minima by 10–20%. Most of these deviations, however, are transfers of economic rent to producers and not economic inefficiency. In particular, economic inefficiencies associated with the use of discriminatory auctions were typically under 0.5%. Furthermore, utilities are likely to pay less for power under auction procedures than using posted prices.

Included with the report are a number of appendices. Some of these present original theoretical derivations. One calculates the effect of revealed second-price auctions in models with subsequent negotiations in which part of the revealed economic rent is captured. Another calculates the optimal selection of quantity to bid when a bid is both a price and a quantity. One appendix presents a workable mathematical procedure for selecting the lowest cost set of bids to a utility. Another presents a precise specification of a sequential bid acceptance procedure and an example of its application. One large appendix contains an extensive discussion of additional issues that would arise if an attempt were made to deregulate all new power generation capacity by removing the technology restrictions (i.e.

small power or cogeneration) on bidders in PURPA power supply auctions. The final appendix illustrates how the interaction of bidders' capacity and bid price decisions can reduce the economic efficiency of discriminatory auctions. (See Fig. 2.)

PLANNED ACTIVITIES FOR FY 1988

We plan to extend this work to consider in detail the additional issues that would arise if auctions were used for all new long-term power generation—not just QF power. We also plan to study auctions held for QF power to observe their effectiveness in practice.

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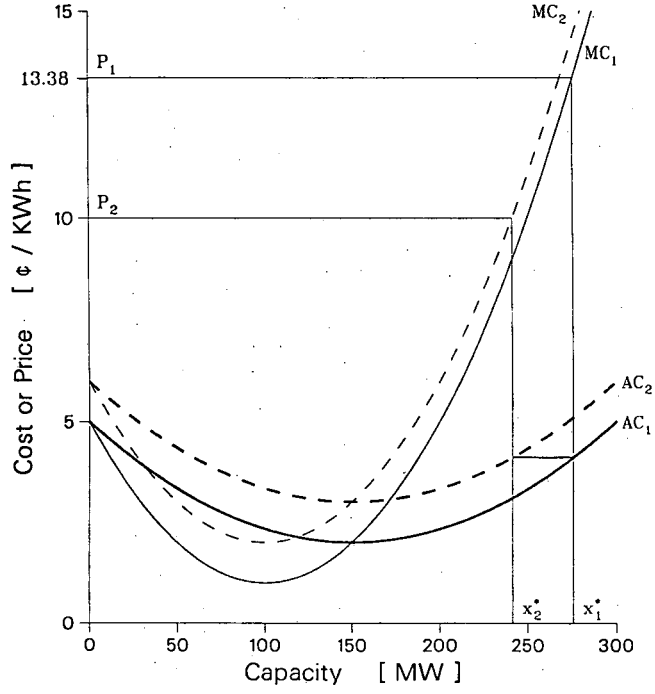

Figure 1. Utility exposure to financial risk from levelized payments in the face of increasing avoided costs. (XBL 878-9071)

BUILDING ENERGY SYSTEMS PROGRAM

INTRODUCTION

The main theme of the Program is the comprehensive simulation, analysis, monitoring, and evaluation of the energy performance of whole buildings, with the emphasis on nonresidential buildings. Many of the projects involve developing and applying the types of comprehensive computer models that enable integrated analyses of heating, cooling, and daylighting system performance. A further activity involves research on absorption heat pumps for solar cooling and gas-driven applications, and analysis of the performance and economics of solar cooling systems.

The Simulation Research Group has two major activities. The first is the maintenance and continued development of DOE-2, a public-domain computer program for detailed, hour-by-hour simulation of energy use in buildings. DOE-2 is in wide use in the U.S. and thirty other countries for design of energy-efficient buildings and for research studies of innovative building technologies. During FY 1987 work continued on adding new capabilities to DOE-2 to enhance its usefulness.

The second main activity of the Simulation Research Group is the development of the next generation simulation software for use in the 1990's and beyond. In collaboration with other groups in the U.S., France, China, and the U.K., a plan has been formulated to create an "Energy Kernel System" consisting of an extensive library of software modules and an executive program which will allow users to produce a wide variety of customized simulation programs. In FY 1987 LBL continued development of the Simulation Problem ANalysis Kernel (SPANK) as the first prototype of the Energy Kernel System.

The Building Systems Analysis Group continued investigation of the energy performance impacts of passive heating, cooling, and daylighting technologies in nonresidential buildings. A simplified correlation was developed to give estimates of the change in energy use resulting from roof-aperture daylighting systems in office buildings. This correlation is suitable for use in a daylighting design tool. Investigations of the ways in which thermal energy storage systems can beneficially impact building energy use continued. The studies conducted in FY 1987 focused on the integration of structural thermal energy storage with the mechanical cooling system.

Under the Solar Federal Buildings Program, a simplified technique for evaluating the long-term performance of daylit buildings based on short-term monitored data was completed, tested, and refined. This work was carried out in collaboration with researchers in the United Kingdom. The project was coordinated with researchers at SERI who are developing thermal performance evaluation methodologies.

Begun in FY 1985, the evaluation of the Institutional Conservation Program, conducted in collaboration with Argonne National Laboratory, was completed in FY 1987. This DOE program provides grants to schools, colleges, and hospitals to identify and implement energy conservation measures (ECMs). The evaluation project was designed to assess the success of the program in serving the needs of the institutional sector. In FY 1987 plans were implemented to collect data through mail surveys and phone interviews. Two additional studies were completed: one was directed at assessing the technical quality of the analysis on which ECM selection is based, and the other estimated the overall impact of the grants on energy use in the institutional buildings sector.

The Active Solar Cooling Project continued research on regenerative absorption heat pumps for high-efficiency solar cooling and heating systems. As part of a joint U.S./Israel effort, computer models are being developed to enable the detailed analysis and design of these and other new types of advanced absorption heat pumps. A parallel task entails simulation and comparative analysis of the expected performance and economics of future solar cooling systems (desiccant and absorption) and conventional vapor compression systems. These analyses keep careful track of all parasitic electrical power requirements as well as the thermal (solar or gas) driving sources.

LBL has also been participating in collaborative projects with other national laboratories involving the monitoring of commercial buildings: assistance to Oak Ridge National Laboratory in developing a protocol for the collection of energy use data for commercial buildings; and assistance to the Solar Energy Research Institute in identifying HVAC monitoring issues for testing the macrodynamic method of determining building thermal energy performance.

Simulation Research*

F.C. Winkelmann, B.E. Birdsall, W.F. Buhl, K.L. Ellington, A.E. Erdem, D.J. Hopkins, J.M. Nataf, O. Nour-Omid, and E.F. Sowell†

The Simulation Research Group (SRG) has the long-term objective of providing the architectural, engineering, and research communities with software tools to assist in the design of significantly more energy-efficient and cost-effective buildings. The ongoing research of the SRG has two main focuses: (1) the development and maintenance of the current-generation benchmark program (DOE-2), and (2) advanced simulation, the development of the next generation of building performance calculation tools (the Energy Kernel System).

As can be seen in Fig. 1, DOE-2 is composed of two major segments: the Building Description Language processor, which accepts descriptions of building components, and the LOADS, SYSTEMS, PLANT, and ECONOMICS processor, which uses building descriptions to simulate building energy performance. Details of the development and structure of the DOE-2 program are available in past annual reports and other published material.[1-18]

The main efforts in the advanced simulation area at this time are the creation of the Energy Kernel System (EKS) and the organization of the simulation development community to enhance collaboration. The EKS will have three main components: software primitives, including a component model library and simulation tools; a software executive to facilitate the construction of simulation programs by allowing general linkage of component models and support models; and a knowledge base that will contain the rules of simulation development and use so as to allow, at a future time, the construction of expert systems for building performance simulation. These three aspects of the EKS will provide the basic tools and information to allow the SRG and other groups to develop the simulation programs of the future. They will also provide a mechanism to facilitate exchange of research results and technology advances, and a basis for integrating performance simulation into computer aided design (CAD) and expert system software.

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†Visiting scientist. Permanent address: Department of Computer Science, California State University at Fullerton, Fullerton, California.

ACCOMPLISHMENTS DURING FY 1987

DOE-2

The SRG maintains a research effort that continues to develop enhanced versions of DOE-2. This ongoing research is divided into three parts: (1) the introduction of algorithm description techniques into the code; (2) the modeling of building envelope components and systems; and (3) the simulation of HVAC equipment and associated control systems. The next version of the program, DOE-2.1D, is scheduled for release to the public in 1988. Its major new features are described below.

User-Defined Functions

Direct user interface with the operation of DOE-2 is currently possible in the LOADS section of the program through the use of the FUNCTION command added during FY 1985. This feature allows direct modification, enhancement, or replacement of DOE-2 calculations without requiring any manipulation of the computer code. Users can write their own algorithms in a FORTRAN-like language and place this information in their building description, along with information indicating how and where these new algorithms are to be used. This is a major step forward in allowing designers and researchers to "fine tune" the simulation program to their specific needs. In the past this was not feasible without a major investment of time. This capability has now been added to the SYSTEMS portion of the program, making it possible for a user to add new HVAC simulation features, such as innovative control schemes.

Generalized Library

In the past it has only been possible to create DOE-2 libraries of materials, envelope constructions, and transfer functions. A new general library feature has been designed which will allow the users of DOE-2 to create custom libraries containing descriptions of any building component or system of components. This will allow definition of libraries containing data which might consist, for example, of standard operation schedules for different building types or of complex component descriptions. Even libraries of whole building descriptions can be created. This new library capability will greatly facilitate use of the program.

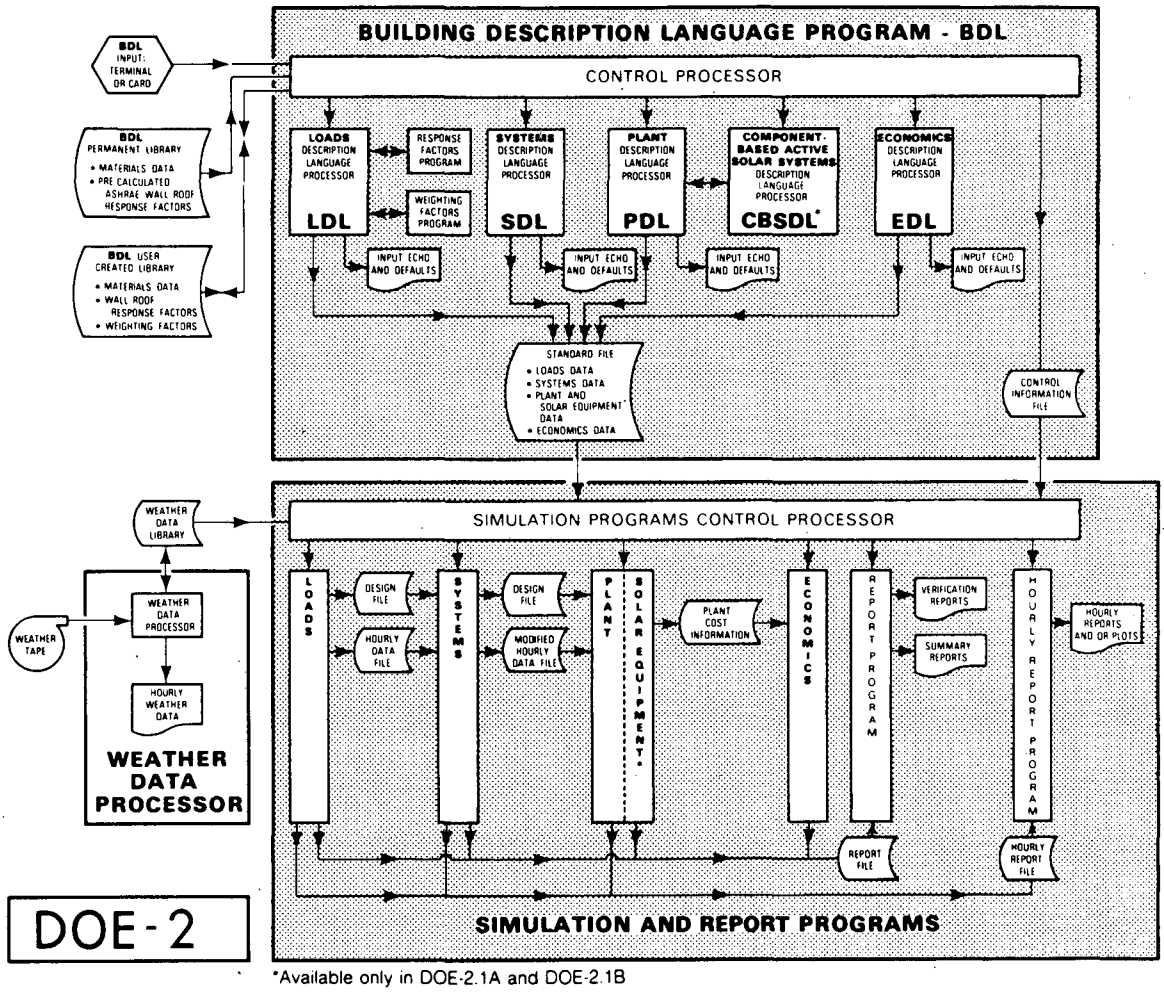

Figure 1. DOE-2 computer program configuration. (XBL 8010-2210B)

Fenestration .

Because heat gain and loss through windows have a large impact on energy performance of most buildings, the DOE-2 window thermal calculations are being improved. This includes (1) an automatic calculation of the shading of diffuse solar radiation by neighboring buildings and by architectural elements such as overhangs (previously only the shading of direct solar radiation was calculated); (2) an improved calculation of infra-red radiation loss from the building envelope to the sky, taking into account atmospheric conditions (atmospheric moisture, cloud coverage) and blocking by architectural obstructions; and (3) an improved calculation of the amount of sky diffuse radiation falling on windows and walls.

Desiccant Cooling

In most climates, occupant comfort during the warmer months requires that room air be dehumidified. Several companies are developing desiccant cooling systems in which a hygroscopic material such as lithium bromide is used to remove moisture from the supply air stream. The desiccant is "regenerated" for further use by drying it with hot air from a gas-fired heater. Gas-fired desiccant systems of this type have the potential for being a replacement for, or a supplement to, conventional electric-driven cooling systems. However, almost nothing is known about the economics of desiccant systems for different climates, building types, and utility rate structures. For this reason, the SRG in FY 1987 (with

funding from the Gas Research Institute via the GARD Division of the Chamberlain Manufacturing Corporation) began development of DOE-2 models that can be used to simulate the performance of a variety of desiccant systems that are on the market now or are under development. Figure 2 shows schematically how a desiccant dehumidification module will be integrated into the air streams of a generic DOE-2 distribution system.

Histograms and Scatterplots

A new statistical analysis package developed by our collaborators in France at the University of Paris-South allows DOE-2 to plot "frequency of occurrence" distributions for any of the program's 200 hourly thermal and climatic variables. The distributions can be in the form of histograms (which show how often particular values of a variable occur) or scatterplots (which show frequency-of-occurrence correlations between two different variables). These plots will make it possible for users to see trends and inter-dependencies which would be difficult to determine from the conventional tabular reports in DOE-2. For example, a scatterplot of cooling coil power vs. outside air temperature (or enthalpy) could be used to study the performance of an economizer cycle.

Advanced Simulation

In recent years, researchers and designers have begun to investigate the use of very advanced technologies in buildings. The search for more efficient building designs has led to components, systems, and whole building structures which are extremely complex and therefore difficult to analyze. Existing programs like DOE-2 were initially conceived in an era when design questions were much simpler than they are today. Thus, there are fundamental limitations in the analysis capabilities of these programs. In particular, techniques have not been developed which allow accurate simulation of the interactions between building envelope components and HVAC equipment and their controls in a generalized, computationally efficient, and easily extendible manner. Analysis of complex designs and advanced technologies requires a substantial jump forward in the capabilities of the next generation of building performance simulation programs. To continue to meet DOE's long-term objective of providing up-to-date and reliable analysis tools, basic research has begun into new simulation techniques. This work will lead to the replacement of DOE-2 with a tool designed to meet the needs of architects and engineers in the 1990's. Several years of negotiations have led to the creation of an international collaborative effort

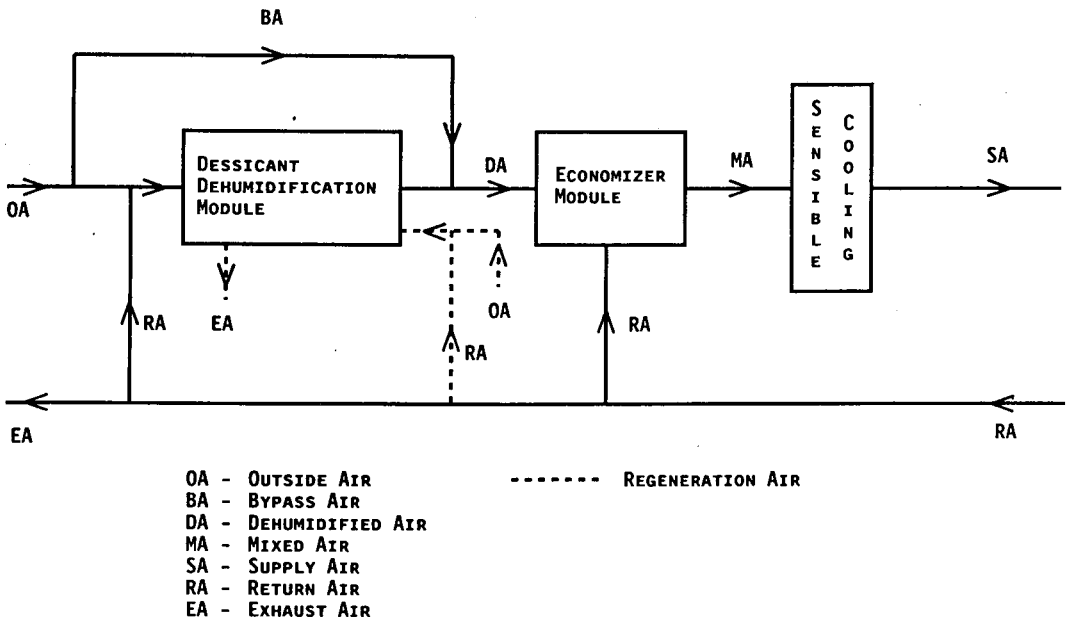

Figure 2. Integration of desiccant dehumidification module into the DOE-2 distribution system. (XBL 8712-5766)

among the U.S., U.K., France, and the People's Republic of China to produce the new software. This effort will provide not only a very significant advance in the building performance simulation field, but also a mechanism for the communication and exchange of results between a diverse community of designers and researchers.

The general goals and structure of the advanced simulation software have been determined.[19-22] The primary goal is to provide a software environment (called the **Energy Kernel System** or **EKS**) for developing new simulation programs which allow a high level of model construction flexibility and which facilitate state-of-the-art developments by making it easy to integrate new techniques with old. Other goals are to permit different modeling approaches, to encourage collaboration among model developers, and to take advantage of emerging software engineering in the area of multiprocessing.

A schematic of the EKS is shown in Fig. 3. The EKS will consist of (1) a library of software modules, or *objects*, representing different building components, physical processes, and mathematical solution techniques, and (2) an executive program, or *harness*, which allows users to link software objects to form customized energy models. The EKS user will first construct a *template* which defines a model as a collection of objects and a set of messages controlling the order of execution of the objects and the flow of information among them. The template is used by the harness to construct the final program in the form of source or executable code.

It is important to note that the EKS is designed for use by model *developers*, not by model users. It is intended to be an efficient way of building simulation models that can be used in a stand-alone fashion or that can be integrated into multipurpose

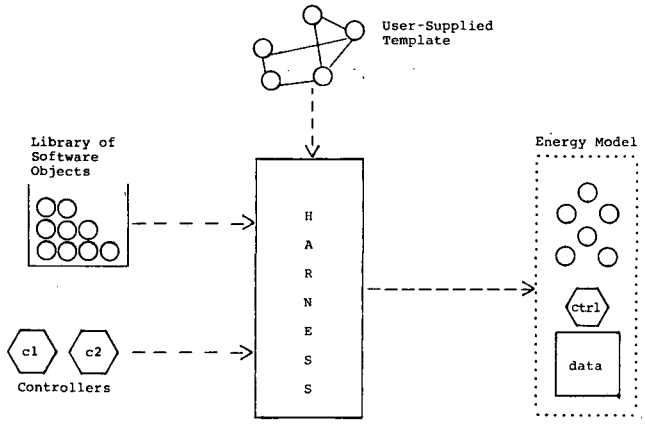

Figure 3. Proposed Energy Kernel System for creating building energy simulation models. (XBL 8712-5767)

environments such as computer-aided design (CAD) systems, expert systems, or energy management systems.

SPANK: A Prototype Energy Kernel System

In FY 1986 the SRG began development of new software called the Simulation Problem ANalysis Kernel (SPANK) as a first prototype of the EKS.[23,24] SPANK views a simulation problem as a network — the nodes represent nonlinear equations, and the lines linking the nodes (called links or arcs) represent variables in the equations. The network representation of a simulation problem is completely equivalent to describing the problem as a set of simultaneous, nonlinear equations. The network representation has the advantage of allowing graph theory techniques to be used to reduce the size of the problem to be solved. The existing version of SPANK only allows algebraic equations, but the next version will handle first-order differential equations.

A simulation problem in SPANK consists of a set of coupled equations. Each equation or relation among variables is known as a "primitive object." Primitive objects may be combined into "macro objects," and primitive and macro objects can be combined into more complex macro objects. Thus modules (sets of equations) that represent complicated physical processes or entities can be built up from simple components. Once the necessary objects, either simple or complex, are defined, the problem description is completed by "linking" the objects together, i.e., by specifying which variables are common to which equations.

Once the simulation problem is defined, SPANK does the rest. The user does not have to choose a computation sequence (that is, write a procedural algorithm in FORTRAN or some other language) that solves the set of equations. SPANK creates the solution sequence in two steps. First, a particular relationship (equation) has to be selected for each variable and inverted to give a formula for that variable. Selecting a relationship to be used in solving for a particular variable is a classic matching problem from graph theory, and algorithms for performing this matching are well known.

Once the matching has been accomplished, the second step is to find a set of break variables, called a "cut set." These variables become the iteration variables in the solution sequence. That is, initial values are guessed, then used to solve for all the variables using the set of relationships, yielding new values for the cut set variables. Then a scheme such as Newton-Raphson iteration is used for choosing the next guess for the cut set.

Most simulation programs, when faced with solving a system of nonlinear equations, simply iterate on all the variables; i.e., the cut set includes all the variables in the problem. One of SPANK's major contributions is to use graph theory methods to reduce the cut size greatly, and thus to effectively reduce the problem size.

At this time the largest practical problem solved with SPANK is a simulation of a constant-volume reheat HVAC system. The model contains 23 equations and 23 variables. The cut set found by SPANK contains 1 variable, a 23 to 1 reduction in problem complexity. The model structure of the SPANK problem description (objects and macro objects) allows a model to be easily comprehended and altered. SPANK inherently allows simultaneity and nonlinearity. Lastly, the use of data flow concepts will allow SPANK to take optimal advantage of multiprocessor machines.

SPANK development continued in FY 1987. The following was accomplished:

(1) Several enhancements were made to improve the robustness of a SPANK simulation, including user-specified starting values to speed convergence and user-specified units on problem variables coupled with automatic program checking of consistency of units on object links.
(2) Object-oriented techniques were developed to allow SPANK to simulate time-dependent processes by integration of first-order differential equations.
(3) A graphical input processor was developed which simplifies input preparation by allowing users to link objects on a VDT screen and display the final network before sending it to the SPANK equation solver.

International Association

A major element of the proposal to develop the EKS was the formation of a new professional association to guide research and development in the building performance simulation field. This organization, called the *International Building Performance Simulation Association (IBPSA)*, officially came into being in January 1987, culminating over three years of meetings and discussions among building professionals. IBPSA aims to promote the science of building performance simulation as a means of improving the design, construction, operation, and maintenance of all types of buildings. Organizers include members of the building industry who use building simulation software, researchers who develop this software, and members of governmental agencies concerned with building performance.

The formation of IBPSA is directly related to the need for new directions in building simulation software foreseen by workers in the field as early as 1983. At a DOE-sponsored conference in Leesburg, Virginia, in the Fall of 1983, industrial users of programs such as DOE-2, BLAST, and proprietary codes met with program developers and researchers to evaluate the status quo and see what new developments were on the horizon or needed. This was followed by two years of discussion and proposals for new sponsored research to address the needs identified at Leesburg. A major milestone along the way was the DOE/ASHRAE-sponsored Building Energy Simulation Conference in Seattle, held in August 1985. Subsequently, a composite proposal for the Energy Kernel System was formulated by an international group working at LBL. That proposal called for a collaborative effort with ongoing guidance provided by an international association. The first meeting of this association, which later became IBPSA, was held in San Francisco in January 1986. After two more meetings and much work in between, IBPSA was incorporated as a non-profit organization in Canada on January 26, 1987. Throughout this process, there has been a growing number of enthusiastic participants, anxious to make IBPSA into a major force in setting future directions in building simulation research and software development.

At its most recent meeting held in Nashville in June 1987, IBPSA embarked on an ambitious program of activities, including plans for a major conference in Vancouver in June 1989. This conference will bring together practitioners and researchers concerned with building energy analysis programs and other aspects of building simulation. In the meantime, there will be a quarterly newsletter and an annual bibliography of related literature. Other projects set in motion include the development of a long-range research priorities list and the formal elections of a Board of Directors and Officers.

PLANNED ACTIVITIES FOR FY 1988

DOE-2

The DOE-2 program will continue to be maintained and supported and its documentation enhanced. The quarterly *DOE-2 User News* will continue to be published. An improved version of the program, DOE-2.1D, will be completed and released to the public.

Advanced Simulation

The SPANK program will be released for outside review after in-house testing of the graphics-based input processor and the dynamic simulation features. Exercises will be carried out to compare SPANK and ZOOM, an advanced simulation program being developed in France. The U.S. and U.K. will begin development of detailed specifications for the Energy Kernel System. Work will continue in the People's Republic of China on new convection calculation techniques for incorporation into the EKS. Work will be completed on three EKS-related projects performed under contract to LBL by other groups in the U.S.: macrodynamic simulation (SERI), a generalized finite element approach for building energy simulation (NBS), and advanced transfer function techniques (University of Wisconsin).

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Building Systems Analysis*

R.C. Kammerud, B. Andersson, B. Birdsall, W.L. Carroll, D. Dumortier, B. Erwine, B. Hatfield, R.J. Hitchcock, B. Lebot, J. Noring, A. Seager, and E. Vine

The Building Systems Analysis Group has been involved in two major types of work during the past year. The first, our more traditional area of work, is nonresidential buildings research. The projects falling under this heading are the development of a methodology for use by energy consultants and engineers to evaluate the energy savings of daylighting applications; the development of a simple set of correlation equations for use in daylighting design tools; and identification of energy-conserving techniques applicable to each of a variety of military building types. The other area of work, newer to this group, is program evaluation. We completed a two-year project to assess DOE's Institutional Conservation Program for its success in serving the needs of the institutional buildings sector.

ACCOMPLISHMENTS DURING FY 1987

Nonresidential Buildings Research

Daylighting Performance Evaluation Methodology Development

Daylighting is an increasingly popular form of solar utilization for energy conservation in buildings, not only because of its economic and energy benefits, but also because of its potential for a positive contribution to the appreciation and enjoyment of buildings. In any passive building, it is important to evaluate the success of the application in terms of energy savings, economic impact, architectural effects, and occupant response. In this methodology development, which is part of the DOE Solar Federal Buildings Program, investigations have been limited to daylighting's impact on energy savings. A methodology for determining energy savings due to solar heating and cooling technologies is being developed by the Solar Energy Research Institute in parallel with this effort.

The ability to make reliable predictions of daylighting performance is dependent upon accurate characterization of two key relationships: (1) interior illumination as a function of the solar resource and the daylighting configuration; and (2) electric lighting energy use as a function of the interior illumination and control of the lights. In FY 1986, during the first phase of this project, a technique based on these two key relationships was developed for evaluating daylighting performance in comparison with a non-daylit building. In short, the procedure uses (1) detailed simulation of the daylighting system, and (2) specific short-term measurements to adjust the simulation, to provide a realistic estimate of the long-term energy savings. The methodology provides a straightforward, reasonably simple, documented means of evaluating daylighting performance for the building owner, designer, or researcher.

FY 1987 saw completion of the second phase, in which the method was demonstrated in a full-scale application. In collaboration with the United Kingdom's Energy Performance Assessment Program, the method was tested on an office building near Birmingham, England. Instrumentation was installed and data collected in the U.K. by a British team with LBL's technical support. The data analysis and evaluation were then performed at LBL with U.K. assistance. Three types of measurements were made: exterior solar radiation, interior illumination, and electric lighting use. These data were used to determine the following under actual operating conditions: (1) interior illumination response to solar radiation, and (2) lighting control response to interior illumination. With this information, both the simulation model that results in illumination levels under varied sky conditions and the model that results in electric lighting use predictions were adjusted to represent properly the *actual* conditions and operation of the building, as shown schematically in Fig. 1. The results showed that the method effectively estimates the long-term electric lighting energy use.

The public domain program SUPERLITE was selected as the basic illumination model. An integrated set of microcomputer software (IBM/PC) was developed for easier and more consistent application of the method. It was refined during the full-scale testing, and it is available for those who wish to use the method.

* This research was supported by the Assistant Secretary for Conservation and Renewable Energy, Institutional Conservation Program Division and the Solar Buildings Technology Division of the U.S. Department of Energy; and by the Electric Power Research Institute and the United States Army Construction Engineering Research Laboratory through the Department of Energy, under Contract No. DE-AC03-76SF00098.

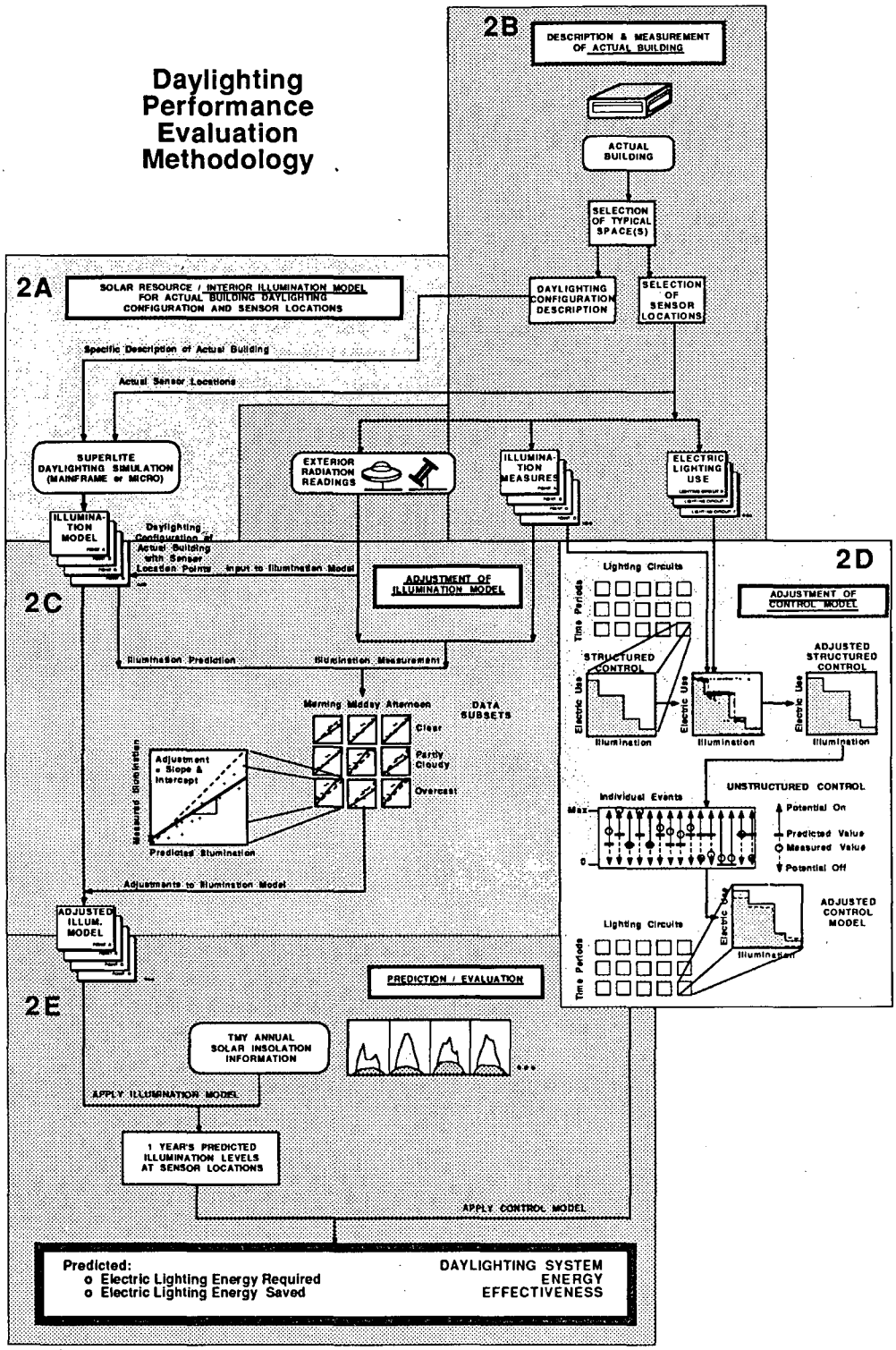

Figure 1. Flow chart of full daylighting evaluation methodology. (XBL 881-56)

Correlation Equations for Daylighting Design Tools

The overall impact of roof-aperture daylighting systems on the energy consumption, and consequently on the utility costs, in office buildings is the result of a complex and detailed set of interactions. An accurate estimate of this effect can be determined only by computer simulations using a detailed hourly energy analysis program that can correctly account for all the interactions. While these simulations can be performed with existing analysis programs, they are typically slow and difficult. However, since design tool accuracy is less important than speed, simplicity, and ease of use, a simplified representation of building energy consumption expressed as a function of the most important building design, operational, and climate factors should be adequate for a design tool. This project is a first effort at developing such simplified correlations for design tool applications.

The general correlation approach utilized a database of office building energy and cost performance to develop simplified expressions for the energy use as a function of selected design, operation, and climate parameters. The database was developed from a series of detailed hourly energy analysis simulations of a prototypical design indicative of current practice. It included parametric variations of a range of roof-aperture daylighting system designs of different sizes and orientations, lighting levels, and climate.

Correlations were derived separately for three components of energy use: (1) lighting electricity, (2) cooling electricity, and (3) heating fuel. Each of the separate correlations was developed by examining the *change* from the annual consumption of a baseline prototype that had no daylighting system, to a modified design which did. This change was expressed as a fraction of the baseline annual consumption of the component.

The combined effect of the individual relative change ratios $\Delta C/C_0$ for cooling electricity, $\Delta L/L_0$ for lighting electricity, and $\Delta H/H_0$ for heating fuel on overall building utility cost performance is:

$$\frac{\Delta\$}{\$_0} = \left(\frac{1}{1+\beta}\right)\left[\left(\frac{1}{1+\alpha}\right)\frac{\Delta C}{C_0} + \left(\frac{\alpha}{1+\alpha}\right)\frac{\Delta L}{L_0}\right] + \left(\frac{\beta}{1+\beta}\right)\frac{\Delta H}{H_0}$$

where

$\$$ represents the total annual building utility costs for electricity and fossil fuel, $\$ = P_E \cdot (L+C) + P_H \cdot H$, for electricity and fuel prices, P_E and P_H, respectively;

C is the annual cooling electricity consumption, L is the annual lighting electricity consumption, and H is the annual fossil fuel consumption for heating;

$\alpha = L_0/C_0$ is the ratio of lighting to cooling electricity consumption for the base case (non-daylit) building; and

$\beta = P_H H_0/P_E(L_0+C_0) = (P_H/P_E)\cdot H_0/(L_0+C_0)$ is the ratio of total annual heating *cost* (price times consumption) to the annual electricity *cost* for the base case (non-daylit) building.

The form of this equation is independent of the actual correlations developed for each of the separate components. The ratios α and β involve only fundamental end-use energy distributions in the base case building and from our database and are dependent on climate. Values for these ratios can be easily determined from information about the specific design of the building and from utility costs. Together with correlation results for the three energy use components, the overall impact of a roof-aperture daylighting system can be easily determined.

Corps of Engineers' Efficient Buildings

Through increasingly stringent energy use standards, the military has significantly reduced energy consumption in the past ten years. Standard building designs are now being developed for a variety of building types. These standard buildings will be used as "templates" for the contracted architects and engineers who design the bulk of military buildings. To ensure that buildings developed from the standard designs can achieve a high level of energy efficiency, the Corps asked LBL to identify the energy conserving techniques that are most applicable to each building type and to develop integrated solutions that can be incorporated early in the design.

Two standard building prototype designs had been developed sufficiently to be analyzed for energy use: Battalion Headquarters and Barracks. A climate analysis was performed to determine the most representative sites for analysis of military building construction. Detailed computer simulation building descriptions were prepared for both buildings to be analyzed with the building energy analysis program BLAST. Basic energy use patterns were characterized for both buildings by simulation of the buildings in different climates. A series of parametric studies was performed, investigating one parameter at a time, to identify the key elements in the energy use patterns.

The work with the Battalion Headquarters building was taken a step further. Using the key parameters already identified, more detailed studies were done to determine the desired ranges of those parameters and to gain a better understanding of their effects and interactions. From these studies, preliminary design guidelines were developed.

Institutional Conservation Program Evaluation Project

The Institutional Conservation Program (ICP) was enacted by Congress in 1978 to provide matching grants to the institutional sector, including nonprofit hospitals, elementary and secondary schools, and colleges and universities, for energy conservation actions. The grants are used to fund energy audits, technical analyses, and installation of energy conservation measures (ECMs).

In 1984 Congress mandated an evaluation of ICP. LBL, in collaboration with Argonne National Laboratory, was chosen to carry out this project. The overall goal of the evaluation project is to identify the most successful measures—both equipment and activities—available to the institutional buildings sector. The evaluation project has two closely related, underlying thrusts, one retrospective and the other prospective. The thrust of the retrospective work is towards examination of (1) energy use data and (2) nonfederal expenditures on ECMs that have resulted from increased awareness of energy conservation potentials engendered by ICP. Through this evaluation we also hope to understand what makes a conservation program successful and how to disseminate this information. Such objectives are prospective and serve as a guide for future conservation efforts.

During the past year, LBL concentrated on the following areas: (1) evaluation of technical audit calculations; (2) analysis of survey results from the higher education subsector; (3) estimates of aggregate energy savings; and (4) analysis of state energy data.

Examination of Technical Audit Calculations

To be eligible for an ECM grant, an institution must have had a technical analysis (TA) of its building(s) performed. This comprehensive analysis results in a written report that describes the building and its energy systems. The report's main purposes are to recommend ECMs appropriate to that building and to serve as a long-term guide for energy management in the institution. A sample of 120 TA reports was examined to determine (1) which calculation techniques are being used to identify ECMs appropriate to the building and (2) whether the energy savings estimates resulting from these calculations are technically sound.[1]

The basic approach was to collect information from the TA report: engineering data about the building and its energy systems, baseline energy use, recommended ECMs, estimated savings with implementation of the measures, and the calculation method by which the savings were determined. This information was used as input to a computer simulation program. The simulations were used to reanalyze the building and the impact of ECMs recommended in the TA report. This study yielded the following observations:

- TA calculations are responsible for only a fraction of the disagreement between actual and predicted savings observed in existing data. Likely sources for the remainder of the disagreement are in design, installation, and operation of the ECMs.
- A wide range of calculation techniques appears in the sample in this study, with a predominance (76%) of simpler, component-based calculations, sometimes modified to account for at least some of the more complex energy issues common in institutional buildings. This observation does not imply that it is common for inappropriate ECM recommendations to be made because of inadequate calculations. Rather, it means that analysts often are limited in (1) the range of ECM options that they can examine, (2) the ability to disaggregate energy use, e.g., to break down electricity use into lighting, cooling, and office equipment, and (3) the ability to account fully for what can be important interactions among ECMs and between the ECMs and the other energy systems in the building.
- In comparison with the reanalyses performed at LBL, the TA reports show a strong tendency to overpredict energy savings, thereby leading to overly optimistic estimates of cost-effectiveness. Figure 2, for example, shows TA-estimated savings versus savings estimated by our reanalysis for envelope measures. In addition, a relatively strong relationship holds between the extent of the overprediction and the type of energy conservation measure under consideration.
- In general, the TA reports do not provide sufficient detail to allow unambiguous determination of the detailed nature of the calculations used and of the specific ECM recommended.
- There is evidence of a lack of sense of scale for energy consumption among end uses in buildings; e.g., what is a typical range of percent of electricity use for lighting in an elementary school, given the

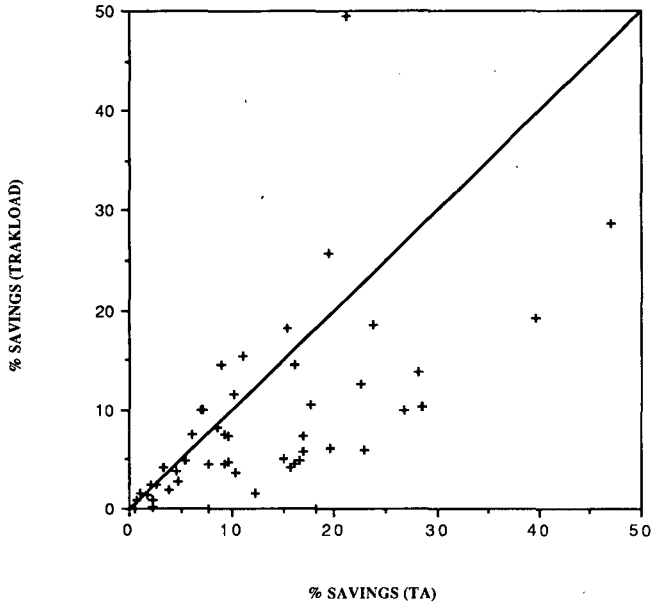

Figure 2. Estimated savings for envelope retrofits: TA vs. TrakLoad. (XBL 876-2989)

other uses of electricity in that school and the other nonelectric energy uses?

We concluded that required use of a particular calculation method is not in order. The appropriateness and accuracy of a given calculation in a given situation depend on how well the calculation represents that measure and how well it accounts for interactions between the ECMs and the other energy systems in the building. It would be more effective to identify conditions and measures under which each type of calculation (1) is adequate in principle, (2) can be adequate if appropriate refinements have been incorporated, and (3) generally is inadequate. To deal with invalid assumptions in TA calculations, we suggest screening reports based on generic energy use information for various types of buildings and also based on detailed lists of invalid assumptions commonly observed.

Survey of Energy Use in Colleges and Universities

The many issues that this evaluation encompasses have required the collection and analysis of new data. Extensive questionnaires were developed for each of the three types of institutions eligible for ICP grants. These questionnaires were sent to institutions that have not participated in ICP as well as to those that have. Information solicited addresses institutional, organizational, and technical issues. LBL analyzed the responses from the higher education subsector.[2] Key findings from the survey were the following:

- Though more than 70% of the survey respondents reported increases in their level of energy conservation effort since 1980, less than 45% reported decreases in energy use, and approximately the same number reported increases. The most commonly reported reasons for changes in energy consumption were (1) changes in building operation, and (2) increases in floor area.
- By far, the most common source of funds used by institutions to purchase energy-saving capital equipment was internal operating and capital budgets, especially by public institutions and ICP participants. Grants ranked second, with substantially fewer institutions using other financing mechanisms. The financing mechanisms that the institutions plan to use to support future energy conservation efforts were ranked in the same order.
- Over 35% of the respondents participated in energy conservation programs sponsored by utilities, and private institutions were more likely to have taken advantage of these programs than their public counterparts. Participation was highest in the West and Southwest.
- The primary motivations for taking energy conservation actions were reported to be the current high cost of energy, the expectation of further cost increases, and utility demand charges or rate structures. The next three most important reasons were related to the institution and its reaction to energy cost factors: cost-containment programs, availability of outside funds, and the support of administration and staff.
- The physical plant director and chief financial officer were reported to be primarily responsible for energy conservation activities in colleges and universities. The most commonly reported information sources for setting overall objectives were the experience of other institutions and professional associations. A wide range of information sources was used in selecting specific measures. However, no information source was dominant.
- In the period between 1973 and 1979, the most common retrofit was the installation of time clock controls, followed closely by caulking and weatherstripping; lighting conversions; heating, ventilation, and air-conditioning (HVAC) system adjustments; insulation; and lighting modifications. Between 1980 and 1986, there was a significantly larger number of measures installed, but they were

very similar in relative frequency to the previous period. In the future (1987–1990), the level of energy conservation activity is expected to remain high; emphasis appears to be changing slightly, with substantial increases in the areas of energy management control systems and lighting retrofits. Continuing a trend developed in the previous two periods, four-year colleges and universities are planning to implement more energy conservation measures than two-year colleges and universities.

- The most effective energy-saving measures were reported to be controls for either the HVAC system or for the lighting system. Other ECMs ranking high with respect to energy savings were envelope measures (e.g., insulation and weatherstripping), lighting measures (e.g., delamping and conversion to fluorescent lights), and heating measures (e.g., boiler replacement). That these measures were most effective is based, in most cases, on the respondents' observations and not on analysis of monitored data.
- Energy conservation efforts have not been trouble-free. Over 50% of the respondents indicated that they have experienced technical problems with the ECMs. Institutions also quite commonly experienced problems associated with occupant behavior (e.g., opening windows in the winter) and with occupant comfort.

Aggregate Energy Savings Estimate

Another facet of the ICP evaluation was an effort to estimate the aggregate energy savings attributable to ICP and the remaining opportunities for saving energy in institutional buildings.[3] The calculation of aggregate energy savings was divided into two parts: the first considers the impact on energy use of ECMs installed with ICP support ("direct savings"). The second considers how ICP may have influenced institutions that have installed ECMs without ICP support. The energy savings in this case are partially attributable to ICP and are referred to as "indirect savings."

The basic approach to determining aggregate direct energy savings is to estimate the savings for each building in each ECM grant, and to accumulate these estimates over all grants. For each building, the estimated energy savings is the value calculated during the original engineering analysis of the building that led to identification of recommended ECMs; this value is entered into the GTS database. In our calculation, this value has been corrected by a factor determined during reanalysis of a sample of 100 of the original technical analyses.[1] Table 1 summarizes the direct aggregate savings results.

The current annual energy savings due to energy conservation measures installed with ICP support is about 3% of the total annual energy use in the institutional sector. The average savings achieved by ICP participants are approximately 12% for educational facilities and 8% for hospitals.

Comparison of the total investment, $1.3 billion, to the total savings to date, $1.9 billion, indicates clearly the cost-effectiveness of the investment. Calculations of aggregate indirect energy savings have been made based on subsector-wide data that allows estimation of (1) the level of ICP-independent retrofit activity and (2) the fraction of the energy savings from these non-ICP retrofits that may be attributable to ICP. By combining the indirect and direct savings, total ICP impacts are determined. Remaining opportunities for energy savings in the institutional building sector are estimated for three scenarios regarding potential performance improvements in

Table 1. Direct energy savings estimates (primary energy, 1987 dollars).

	Schools	Colleges	Hospitals	All[a]
Number of ECMs installed	45,483	14,807	9,645	69,935
Total ECM installation costs (million $)	522	349	524	1,386
Total energy savings (trillion Btu) (ICP start through 1987)	91	88	137	317
1987 annual energy savings (trillion Btu/yr)	19	18	28	64
Total cost savings (million $)	670	508	745	1,924
1987 annual cost savings (million $/yr)	132	102	153	387

[a]Numbers may not total correctly due to rounding

existing buildings. The performance levels are: (1) the average savings achieved by ICP participants to date in each subsector (minimum potential); (2) those reflected in good design practice for new buildings currently being built in each subsector (maximum economically feasible potential); and (3) a benchmark reference that ignores economic feasibility, for savings believed to represent the technical limit in performance for buildings in each subsector. A summary of the indirect savings and remaining opportunities is shown in Table 2; for completeness, direct savings are also shown.

Key conclusions from indirect savings and remaining opportunities calculations are:

- Indirect savings are substantial, ranging from about 40% to 80% (depending on subsector) of the direct savings; this implies that the ICP program has had substantial influence on non-ICP retrofit activities in all institutional subsectors.
- A broad range can be defined for the remaining opportunities for energy savings in each of the subsectors, depending on the assumptions as to the attainable performance improvements. There is substantial variation across the subsectors in the magnitude of the remaining potential relative to either the ICP or total energy conservation impacts to date.
- When the cumulative impact of all institutional sector retrofit activities is considered, the pool of remaining opportunities for continued retrofitting of the existing stock at past levels of cost-effectiveness or payback are declining. Increasingly, the energy consumption characteristics of the institutional subsectors are being determined by previously retrofitted and newly constructed buildings. Further retrofits, to be competitive, must be at least as attractive as the economic returns from other investments available to the institution.

Energy Use in Minnesota Schools

An analysis was made of energy consumption data for schools in Minnesota during the 1970s and 1980s.[4,5] We estimated energy savings for individual schools and for the entire group of Minnesota schools participating in ICP. The actual savings, based on an analysis of pre-retrofit and post-retrofit energy usage, was about 5%. We conclude that existing energy conservation efforts are producing incremental improvements in overall energy performance in Minnesota schools, amounting to substantial savings in the aggregate. Moreover, actual energy savings may be substantially larger than the 5% found in our analysis: a significant fraction of the savings may be offset by other physical or functional changes that often tend to increase energy use in the institution. Other conclusions reached by this study are:

- Annual variation in energy use for a particular institution can be quite large and may mask the energy savings of ECMs. Detailed information on the causes of variation in energy use is necessary for isolating the energy effects of ECMs.
- As shown in Fig. 3, there was no significant difference in the energy use intensities (kBtu/ft^2), or EUIs, of ICP participants and nonparticipants in Minnesota. Accordingly, the unpenetrated stock of buildings represents a large audience for continued energy conservation efforts.

Table 2. Indirect savings and remaining opportunities (trillion Btu/yr).

	Schools	Colleges	Hospitals
Impact of past ICP activities			
Direct savings	19	18	28
Indirect savings	8	14	15
Total ICP impacts	27	32	43
Total impacts not attributable to ICP	24	33	7
Total energy conservation impacts to date	51	65	50
Remaining Opportunities			
Minimum	67	47	23
Maximum Feasible	197	83	92
Technical Limit	360	306	253

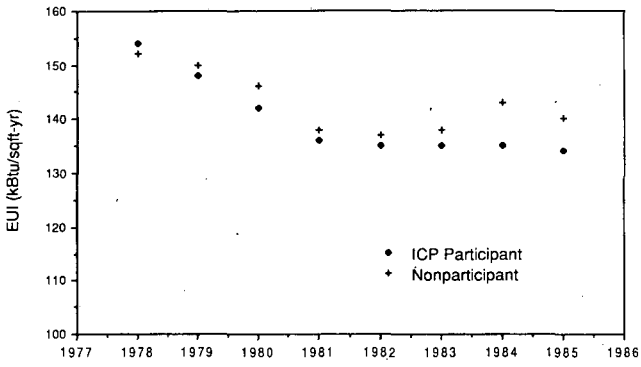

Figure 3. Area-weighted mean EUI for Minnesota schools. (XBL 881-55)

PLANNED ACTIVITIES FOR FY 1988

Nonresidential Buildings Research

Further testing of the daylighting evaluation method will be performed. The method will be refined and enhanced by (1) testing with atria and other daylighting configurations, and (2) extending the method to qualitative evaluation of the daylighting system in addition to estimation of energy use.

To reach a stage in the Corps of Engineers project in which useful, distilled information can be given directly to the designers, several steps will be taken with the Battalion Headquarters. First, comfort effects will be evaluated, especially with respect to thermal mass and floor insulation. Second, innovative, integrated, energy-conserving solutions will be developed and tailored for each of the ten climates. Finally, we will work with Corps personnel to develop information for release to the designers and the Corps design reviewers.

A new project in FY 1988 is development of a methodology for cool storage sizing. In the first phase, simulations will be carried out to examine hourly and daily cooling capacity requirements for prototypical office and retail buildings in Dallas and Chicago. Analyses will be conducted to provide a better understanding of the cooling coil load profile. In the second phase, we will characterize peak conditions and identify associated cooling requirements for a broader range of building types. Parametric analyses will be carried out to examine the relationship of peak cooling requirements and building design variables. The components of the second phase will be synthesized to produce the pilot sizing methodology. We also plan to develop and document a mathematical model for storage sizing.

Institutional Conservation Program Evaluation Project

Although plans have not been finalized, several areas of research are under consideration. One major area relates to recommendations resulting from the examination of technical audit calculations. Possible projects include (1) examining reported ECM problems in depth, (2) documenting energy use scales for institutional buildings, (3) developing calculation screening tools for use by TA analysts and state energy offices, and (4) developing ECM "menus" for small schools. Another major area is activities based on analysis and interpretation of the aggregate data for the institutional sector. Candidate activities are (1) forecasting and evaluating impacts of energy conservation programs and (2) determining economically optimal penetration strategies.

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Active Solar Cooling*

M. Wahlig, J. Rasson, M. Warren, and I. Parmaksizoglu

The purpose of this project is to make major contributions to the technology base necessary for solar energy to become a viable option for the cooling of buildings. This project has two major tasks: (1) research on improved absorption cycles for high-efficiency active solar cooling and heating systems and (2) systems analysis of active solar cooling and heating systems to establish operating requirements, research needs, and thermal performance of current and advanced space conditioning systems. In addition, LBL has been assisting the DOE Solar Buildings Program in planning and coordination activities for the solar cooling part of the research program.

The objective of the absorption cycle research is to achieve a significantly higher conversion efficiency than is possible using other approaches to solar cooling and heating of buildings. In recent years, research has concentrated on *regenerative* absorption cycles, a technological approach that attains high efficiency by more closely approximating (than do other cycles) an ideal Carnot cycle. Early analytical calculations predicted that a double-effect regenerative (2R) absorption-cycle chiller would operate at about 55%, and that a single-effect regenerative (1R) absorption chiller would operate at about 70 to 75%, of the ideal Carnot coefficient of performance (COP). The 2R chiller was built and tested, and it attained the predicted performance, as reported in last year's Annual Report. In parallel, work was begun on developing an analytical capability to model in detail the expected performance of advanced absorption cycles.

The objectives of the systems analysis activities are: (1) to perform systems simulation and analysis of active solar absorption and desiccant cooling/heating systems to establish the operating requirements and thermal performance of current and advanced space conditioning systems; (2) to develop methods to analyze different cooling systems in a common comparative framework; and (3) to evaluate by computer simulation the impact of system controls and control strategies on annual energy savings of advanced solar-driven heating, ventilating, and air conditioning systems.

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ACCOMPLISHMENTS DURING FY 1987

Absorption Cycle Research

As part of a joint U.S./Israel project on solar cooling, LBL and the Technion (in Haifa, Israel) are developing techniques to model and simulate the performance of high efficiency absorption chillers/heat pumps, enabling prediction of the performance of solar cooling and heating systems using these chillers/heat pumps. LBL is adapting the public-domain process flowsheet ASPEN (Advanced System for Process Engineering) for this purpose. By the end of FY 1986, the detailed modeling of the 2R regenerative absorption heat pump had been accomplished; this represented the first successful application of the ASPEN program (or any program) to model in detail a fairly complex absorption heat pump.

Early in FY 1987, a sensitivity analysis was conducted of the 2R chiller performance as a function of condenser/absorber temperature, generator temperature, and evaporator temperature. The results were accurate and reproducible, indicating that the ASPEN program and the ammonia-water thermodynamic model are capable of converging to a unique solution for all operating conditions.

As a cross check, ASPEN and the model under development at the Technion were both used to simulate a single-effect ammonia-water absorption chiller. The two models gave essentially identical results. ASPEN has an advantage in being a more robust solution method: it allows relaxed tolerances for initial guesses to ensure program convergence.

Attention was then turned to adapting ASPEN to the more difficult task of modeling the 1R regenerative absorption cycle. The 1R cycle is more elegant yet more complex than the 2R cycle; it comes closer to matching an ideal Carnot cycle, with less hardware than the 2R cycle, but at the expense of additional flow pathways. Therefore, its modeling is a greater challenge. Modeling of the regenerator component, which is a multistream heat exchanger, was a major effort, as models for this type of component do not exist in ASPEN. The component was modeled as a set of parallel vapor-liquid rectification columns, with external heat exchange. One geometry option for this component model was tested successfully by the end of the fiscal year, and work on this method of modeling the 1R cycle will continue in FY 1988.

In parallel, it was decided to try to develop a simultaneous-equation solution technique for the 1R cycle using the algebraic equation solver HYBRID.

The sensitivity of the refrigerant enthalpy to the ammonia concentration in the evaporator often leads to convergence failure for simultaneous solution methods. This difficulty was overcome by separating the cycle convergence criteria from the equation-solver convergence criteria. This technique was then used to solve sets of linear algebraic equations that simulate 6-, 5-, 4-, and 3-pressure-step 1R cycles, generating performance maps for a range of operating conditions. Although this HYBRID solution method is very useful for "design case" analysis, off-design analysis requires the more rigorous solution approach only possible at this time using an iterative solution technique like ASPEN.

Systems Analysis

As part of the Active Solar Cooling Program, LBL has undertaken a comparative analysis of the technical performance of future ventilation mode desiccant systems with proposed advanced absorption and with conventional vapor compression systems.[1,2] A common framework has been developed for direct comparison of very different cooling technologies building on previous work.[3] Psychrometric analysis is used to determine the performance of the supply air cooling system. Energy for distribution of air is explicitly determined from component and duct pressure drops assuming a 50% fan efficiency. The parasitic energy requirements of other air side components are also calculated. For those systems with cooling coils, the chiller is modeled to meet the cooling coil load, and indirect or regenerative evaporative cooling is also modeled. The comparison of such widely differing technologies as open cycle solid desiccants and absorption cooling systems requires careful evaluation of the cooling supply air delivery system.

Our approach has been to use a standard DOE-2.1C simulation of a commercial building to develop the cooling load information. The building chosen for study is a medium-sized, 50,000 ft^2 (465 m^2), commercial office building which has been simulated using Weather Year for Energy Computation (WYEC) data in five cities: Miami, Atlanta, Fort Worth, Phoenix, and Washington, DC.

System hourly reports were evaluated and certain parameters were binned as a function of outdoor conditions. In particular the supply and return air conditions (temperature, humidity, flow volume) and the fan power are essential to determine the amount of cooling delivered to the space, which usually differs from the heat extraction rate at the cooling coil. The average conditions at each outdoor temperature and humidity bin are then used to perform a psychrometric calculation of the supply air delivery system for the different technologies being compared. The control strategy for the system must be modeled explicitly.

The performance of the system over an entire year is calculated by multiplying the energy used for each of the 30 to 40 bins by the number of hours of occurrence and then summing over all bins. A computer program, BINSYS (Bin Systems), has been written to evaluate the performance and to aggregate the results for an entire year.

The output from the program is the electrical power consumption for air distribution, parasitics, chiller, and heat rejection; the thermal energy input required to run the process; and water consumption of each component. If monthly bin-hours are provided, then the monthly total thermal energy input and the average input temperature can be calculated to evaluate the utilizability of solar energy to drive the cooling process.

Both advanced absorption and ventilation mode desiccant systems show promise of annual performance which is competitive with modern centrifugal chillers. Because ventilation mode desiccant systems can provide colder, dryer air much of the year, on an annual basis they can have lower fan power requirements than do comparable coil-based systems. Advanced absorption systems operated at 140 C have a performance comparable to real desiccant systems. The ability of solar energy to displace fossil fuels to operate absorption and desiccant systems will depend critically on the annualized cost of solar energy being competitive with the fossil fuel alternatives.

Cooling Technology Integration

A number of planning, review, and coordination activities were performed in FY 1987 in support of the overall DOE solar cooling program. A U.S./Israel Workshop on Absorption Technology was organized and held. Meetings were held that led to setting the research agenda for the second year of the joint U.S./Israel project on solar cooling. A report on the status of the DOE solar cooling program was prepared and distributed for review. A planning document was written to assist DOE in preparing a Multiyear Technology Plan for solar cooling. It is anticipated that similar activities in support of the DOE solar cooling program will continue in FY 1988.

PLANNED ACTIVITIES FOR FY 1988

Work will continue during FY 1988 on modeling the 1R cycle using the ASPEN solution method, and calculations using the HYBRID solution method will be used for comparison. Once the 1R cycle has been successfully modeled, plans call for using these techniques to model other advanced absorption cycles that have potential for use in future solar cooling systems.

Comparative analysis of the performance of advanced absorption and desiccant solar cooling systems will continue during FY 1988. The program BINSYS will be refined and applied to (1) incorporation of the most appropriate heating-mode capabilities into the leading cooling system models for desiccant and absorption systems, so that realistic analyses can be made for annual performance in a variety of climatic regions; and (2) coupling of the cooling and heating elements of the systems with appropriate solar collector subsystems, thereby modeling complete solar cooling systems.

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Monitoring of Commercial Buildings*

M. Warren

LBL has a number of building energy research projects sponsored both by DOE and others that address technical and programmatic aspects of performance monitoring of commercial buildings, including the Building Energy-use Compilation and Analysis (BECA), Passive Systems and Materials, Solar Federal Buildings, and Active Solar Cooling.[1-5] As the result of this experience, LBL has recently participated in two projects: the Development of Commercial Buildings Monitoring Protocol, supported by Oak Ridge National Laboratory (ORNL), and HVAC Monitoring in Commercial Buildings, supported by the Solar Energy Research Institute (SERI).

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ACCOMPLISHMENTS DURING FY 1987

LBL has participated with ORNL as part of the Building Energy Retrofit Research Program in the draft and review of a commercial monitoring protocol guideline. The goal is to develop a consensus document which will assist researchers undertaking the study of commercial building energy use to collect information that will allow comparison of buildings across different studies. The developing protocol guideline has been prepared by ORNL and has been actively reviewed by LBL and others.

LBL has been working with SERI as part of the Solar Federal Buildings Program to identify the HVAC issues important for the macrodynamic methodology for determining the building thermal response.[6] During FY 1987 LBL identified a building, developed a measurement plan, assisted with instrumentation of the building, and analyzed the data from the Washington Association of Counties Building in Olympia, WA. Data from the building has been automatically collected once a day and periodically analyzed on a microcomputer. The focus of the analysis is to understand the performance of the heat pump and the variable volume and temperature, VVT, air distribution system using temperature, electrical energy use, and air flow measurements. A paper describing the work is in preparation.[7]

PLANNED ACTIVITIES FOR FY 1988

Depending on availability of funding, LBL plans to continue participation in the monitoring protocol development work and to work with other laboratories in the use of monitoring to understand building energy performance.

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Active Solar Cooling

Building 90, Room 2024
Lawrence Berkeley Laboratory
Berkeley, CA 94720

1987

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Monitoring of Commercial Buildings

Order from Active Solar Cooling

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WINDOWS AND LIGHTING PROGRAM

INTRODUCTION

Over 30% of all energy used in buildings is attributable to two building elements, windows and lighting. Together they account for annual consumer expenditures of over $50 billion. Each affects not only energy use by other major building systems but also comfort and productivity, factors that have a far greater influence on building economics than direct energy consumption alone. Windows play a unique role in the building envelope, physically separating the conditioned space from the world outside without sacrificing vital visual contact. Lighting systems make it possible to conduct any task of any visual difficulty anywhere in the indoor environment, and at the same time define the luminous qualities of the indoor environment. These two building elements are thus essential components to any comprehensive building science program.

Despite the important achievements in reducing building energy consumption over the last decade, significant additional savings are still possible. These will come from two complementary strategies: 1) better building designs that effectively apply existing technology and extend market penetration, and 2) new advanced technologies to increase the savings potentials with each application. Both the Windows and Daylighting and Lighting Systems Research groups have made substantial contributions in each of these areas. The ongoing research described in the annual summary aims to further advance achievement of these goals.

The Windows and Daylighting Group focuses on developing the technical basis for understanding the energy-related performance of windows. If the flow of heat and light through windows and skylights can be properly filtered and controlled, these building elements can outperform any insulated wall or roof component and provide net energy benefits to the building. The group's investigations are designed to develop the capability to accurately predict net fenestration performance in residential and commercial buildings. Simulation studies, field measurements in a mobile field test facility, and building monitoring studies help us to understand the complex tradeoffs in fenestration performance. The Group's three major project areas are optical materials, fenestration performance, and building applications and design tools.

In our studies of optical materials and advanced concepts, we develop and characterize thin-film coatings and other new optical materials that control radiant and thermal flows through glazings. Innovative concepts for large-area envelope enclosures are studied. The program helped accelerate the development and market introduction of windows incorporating high-transmittance, low-emittance coatings for R3-R5 windows. If they sell as currently anticipated, they will save consumers over $3 billion annually in heating bills alone.

Our research on window performance aims to develop new analytical models and experimental procedures to predict the thermal and solar-optical properties of the complex assemblies of glazing materials and shading devices that comprise complete fenestration systems. Thermal performance models are being validated with the Mobile Window Thermal Test (MoWiTT) Facility, now collecting data at a field test site in Reno, Nevada. This unique facility combines the accuracy and control of lab testing with the realism and complexity of dynamic climatic effects. LBL daylighting studies employ a unique 24-foot-diameter sky simulator for testing scale models under carefully controlled conditions, and new experimental facilities for measuring the photometric and radiometric properties of complex fenestration systems.

Building applications studies and design tools help us to understand the complex tradeoffs in fenestration performance as a function of building type and climate. In nonresidential buildings major reductions in electric energy use and peak electric demand can be achieved if the tradeoffs between daylight savings and solar-induced cooling loads are understood. We are developing concepts for an Advanced Envelope Design Tool using new imaging techniques and expert systems.

The research of the Lighting Systems Group is divided into three major areas: advanced light sources, building applications, and impacts on health and visibility.

Our light source research is concerned primarily with developing new concepts for efficiency converting electrical energy into visible light. Areas of interest include mechanisms for reducing the ultraviolet self-absorption in gas-discharge lamps and

the excitation of plasma gas at ultrahigh frequency ranges (approximately 10^9 hertz). Both hold the promise of a more reliable and more efficient conversion of energy into light.

The building applications research concentrates on the design of lighting systems and the effective use of lighting controls, and their interaction with a building's HVAC system.

Research in visibility impacts is focused primarily on gaining basic information needed to define lighting conditions that enhance productivity in a cost-effective manner. It also seeks to determine any possible undesirable visual effects, such as excessive fatigue, associated with using modern office equipment such as visual display terminals in an advanced lighting environment.

Our studies of health impacts extend electric lighting research to a wider class of human activities. In specially designed experimental rooms, conditions can be varied, and nonsubjective responses to lighting variables can be measured by sensitive instrumentation.

The Lighting Group's successes include advancing the development of high-frequency solid-state ballasts for fluorescent lamps and the invention of a new high frequency surface wave lamp with 30% better efficiency than the common fluorescent lamp. A 2-year test of solid-state ballasts in a large office building showed an electricity savings of 40%. Scaled to the entire country, this represents an annual savings of $5 billion. The energy-efficient surface wave lamp promises major reductions in energy use with considerably longer lamp life.

Windows and Daylighting*

S.E. Selkowitz, D. Arasteh, D.L. DiBartolomeo, R.L. Johnson, H. Keller, J.J. Kim, J.H. Klems, C.M. Lampert, K. Papamichael, M.D. Rubin, R. Sullivan, and G.M. Wilde

Approximately 20% of annual energy consumption in the United States is for space conditioning of residential and commercial buildings. About 25% of this amount is required to offset heat loss and gain through windows. In other words, 5% of U.S. energy consumption—the equivalent of 1.7 million barrels of oil per day—is tied to the performance of windows. Fenestration performance also directly affects peak electrical demand in buildings, sizing of the heating, ventilating, and air-conditioning (HVAC) system, and the thermal and visual comfort of building occupants.

The aim of the Windows and Daylighting Group is to develop a sound technical base for predicting the net thermal and daylighting performance of windows and skylights and to accelerate development of new technology that will improve performance and reduce energy use. The group's work will help generate guidelines for design and retrofit strategies in residential and commercial buildings and will help develop new advanced computer-based tools for building design.

One of our program's strengths is its breadth and depth: we examine energy-related aspects of windows at the atomic and molecular level in our materials science studies, and at the other extreme we perform field tests and *in-situ* experiments in large buildings. We have developed, validated, and use a unique, powerful set of computational tools and experimental facilities. Our scientists, engineers, and architects work in collaboration with researchers in industry and academia.

To be useful, the technical data developed by our program must be communicated to design professionals, industry, and other public and private interest groups. We publish our results and participate in industrial, professional, and scientific meetings and societies, national and international, to ensure that our research results are widely disseminated.

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Buildings and Community Systems, Building Systems Division, and Office of Solar Heat Technologies, Solar Buildings Division, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Our research is organized into three major areas:

- Optical Materials and Advanced Concepts
- Fenestration Performance
  - —Thermal analysis
  - —Daylighting analysis
  - —Field measurement of performance
- Building Applications and Design Tools
  - —Nonresidential buildings
  - —Residential buildings
  - —Design tools

OPTICAL MATERIALS

Significant reductions in energy consumed by buildings will come not only from better building design, but also from the development and introduction of new glazing materials. Since the inception of our program in 1976, we have worked to identify, characterize and develop promising new optical materials to assist industry with developing the next generation of advanced fenestration systems. We also provide scientific coordination for DOE-funded research projects at universities, private-sector firms, and other national laboratories, and work to transfer our research results to the private sector.

In 1976, we made the development of low-emittance (low-E) coatings a major program objective. DOE-supported research has accelerated market introduction of new high-performance low-E window systems. Several small firms began offering commercial products in 1982, and by 1985 most of the largest glass and window manufacturers offered low-E products. The use of low-E coatings in a conventional double-glazed window provides better thermal performance than triple glazing and makes a lighter and more compact window. In the long term this coating technology could produce windows having heat transfer values as low as those of insulating walls. On an annual basis such windows should outperform the best insulated wall.

CHARACTERIZING COATED GLASS AND PLASTIC SUBSTRATES

To predict the performance of complex window systems, we must accurately know the optical properties of their coatings and glass and plastic substrates. Until recently, scientists did not fully understand these properties for even the most common varieties of glass used in windows. We have completed work on standard clear glasses, glasses having absorbing additives, and high-purity glasses. Our results were summarized in a paper that includes a complete set of optical constants from the near ultraviolet through

the little-studied far infrared for all common window glasses.[1] We also provided spectrally and directionally averaged bulk properties for calculating solar and thermal radiative heat transfer through windows.

Accomplishments During FY 1987

With the increasing marketing of low-E window systems, there is a concern that emittance be properly measured, calculated, and specified. Normal emittance can be measured in a spectrophotometer, but hemispherical values are required for thermal analysis. We previously developed a procedure to determine the hemispherical emittance of a low-E coating if the normal emittance is known. This correlation, shown in Figure 1, was adopted by industry groups as a standard calculational procedure. We also participated in a series of industry-sponsored round-robin emittance measurements.

Planned Activities for FY 1988

We will continue measurement and analysis of coated glazings, seeking generalizable relationships between simple, measurable parameters and the more complex angle-dependent and spectrally dependent behavior of specific coatings. We will also continue collaborative work with an industry group developing voluntary standards for measurement of emittance.

DURABLE LOW-EMITTANCE COATINGS

Since 1976 we have contributed to the development of low-E window coatings that transmit sunlight but reflect infrared radiation, thus suppressing radiative heat transfer. Commercially available coatings based on vacuum-deposited metal-dielectric multilayer films have satisfactory optical properties and a low emittance value, 0.1-0.15, but are not sufficiently durable to be used in nonsealed glazings. Pyrolytic films deposited directly on glass in the float process are more durable but typically have a higher emittance, 0.35, and thus lower energy savings potential. We approach the problem by identifying materials with good intrinsic durability and then attempting to improve the emittance and solar-optical properties.

Accomplishments During FY 1987

We began by studying the titanium oxynitride (TiN_xO_y) system, producing these gradient-index coatings first by plasma-assisted chemical vapor deposition (PCVD) and later by sputtering. To achieve better film properties in FY 1987, we switched to a multilayer coating design, TiO_2-TiN-TiO_2. By varying the TiN thickness and deposition parameters, we were able to obtain coatings with visible transmittances and emittances approaching those of some of the pyrolitic coatings (Figure 2). The coatings were characterized by electron microscopy, Auger electron spectroscopy (AES), and Rutherford backscattering (RBS), in addition to complete optical characterization. Detailed data on deposition parameters and coating properties were developed for industry with the objective of getting our results duplicated on production-scale sputtering machines. We are discussing with developers of sputtering systems the feasibility of modifying existing systems to

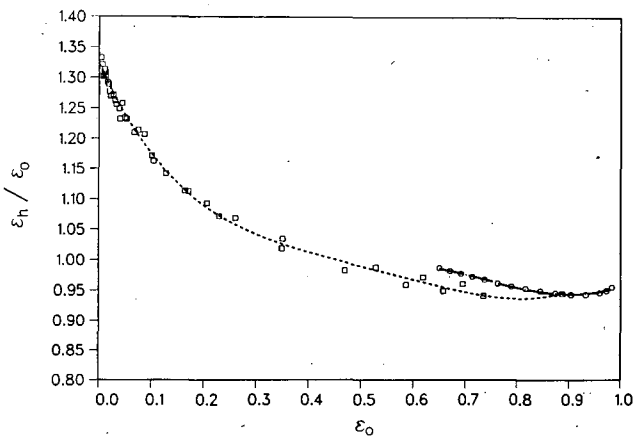

Figure 1. Normalized hemispherical total emissivity versus normal emissivity. Solid curves approximate (□) metals and coatings on glass, and (0), dielectric substrates. (XBL 876-2803)

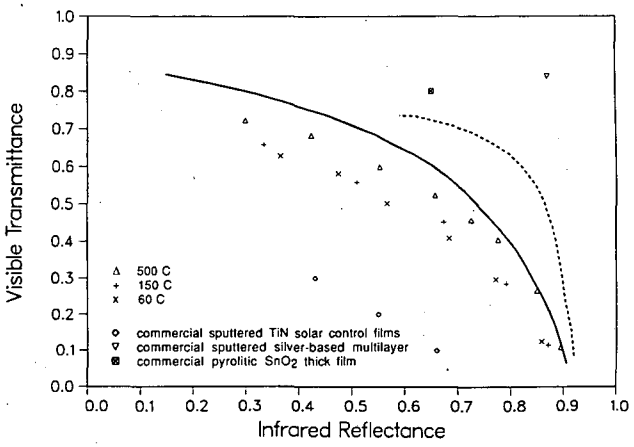

Figure 2. Calculated solar transmittance versus infrared reflectivity of TiN films (solid line) and TiN / TiO_2 multilayers (dotted line). Properties of TiN films deposited at three different substrate temperatures are also shown. (XBL 884-1468)

allow for heating the glass substrate, which is required for deposition of our best coatings.

Planned Activities for FY 1988

We expect to continue collaboration with industrial coaters who are interested in manufacturing TiN-based coatings. Limited durability testing may be undertaken. We have started work on transparent, diamond-like, hard carbon coatings that could serve as a protective overcoat for other optically important coatings.

LOW-CONDUCTANCE GLAZINGS

With the commercial success of R3-R4 low-E windows, the next major challenge lies in developing high-R (R6-R10) glazings. In 1985 we developed a new concept for a high-R window that can be manufactured using existing technology. A DOE patent application was filed and subsequent research and development of the concept was sponsored by the Bonneville Power Administration (BPA).

Our high-R window is based on an innovative modification of conventional triple glazing. Two low-E coatings (emissivities < 0.10) are placed on surfaces facing each of two sealed gaps. To reduce conductive heat transfer and achieve optimum thermal performance, a Krypton or Krypton/Argon gas fill is used instead of all Argon. This allows us to keep the gap widths small and produce a unit with an overall width of 0.75-1.0 inch, small enough to be used in conventional sash and frame designs.

Accomplishments During FY 1987

During the past year, computer analyses and lab and field tests have shown that a window with an overall effective R-value of R6-R8 (R8-R10 center of glass) can be commercially produced using low-E coatings and krypton-based gas fills. At gap widths of 0.35 inch, the differences between 100% Kr and 50/50 Kr/Ar are small, but the difference between using two standard low-E coatings (emissivity of 0.15) and two high-performance low-E coatings (emissivity of 0.05) is large. Proposed window designs would therefore concentrate on using the better low-E coatings available today with emissivities under 0.10 (Figure 3).

In small quantities, pure Krypton is too expensive to use in gas-filled windows. However, the prospects for much lower prices for large quantities of "crude" Krypton are good. Improved filling techniques under development will reduce gas waste. At present very little data exists on the expected lifetime of gas fills in insulated glazings. European experience

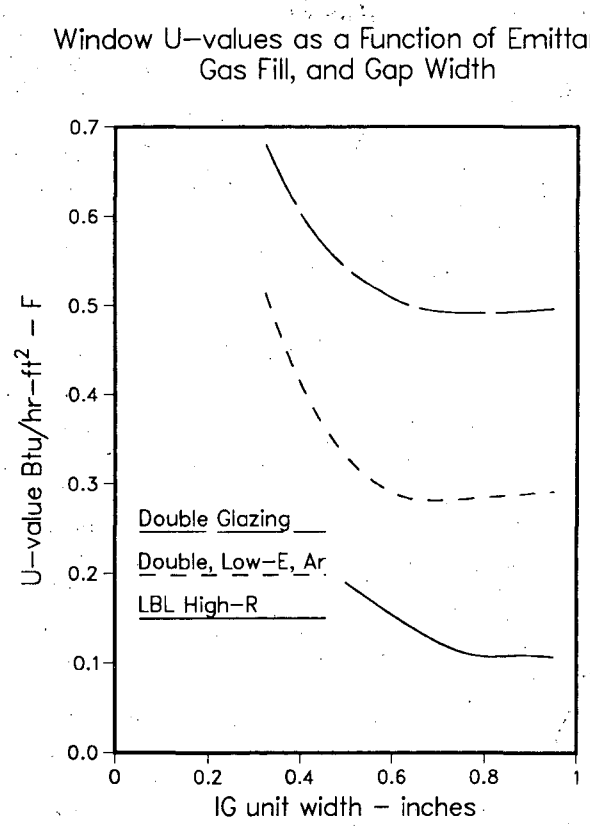

Figure 3. Window U-values as a function of insulated glass unit width for conventional double glazing; low-E (e = 0.15), Argon-filled double glazing; and an LBL high-R design (two e = 0.05 coatings, two krypton-filled gaps). Nominal 1/8-inch glass assumed for all glazing layers. (XBL 884-1469)

suggests that with the proper sealant and sealing procedure, gas leakage should not be a problem. Argon has been the primary gas examined for this purpose; Krypton's rate of diffusion should be significantly lower because of its comparatively larger molecular size.

A finite-element computer analysis showed that the structural stresses in such a window system should be within design constraints. A window with thinner Krypton-filled gaps will create less stress and smaller deflections than a wider Argon unit. Future work will address the thermal bridging effect from the use of conventional metal spacers in a highly insulating window, and gas diffusion rates through alternative nonmetallic spacers.

Planned Activities for FY 1988

We will continue to study specific technical problems, such as the influence of different frame and edge materials on overall U-values, gas retention, gas-filling processes, gas costs, center glazing-

layer materials and structural performance. Second-generation technical proof-of-concept prototypes of the most promising options will be built and field tested. In these field tests, we hope to show that high-R glazings can outperform insulated walls. We expect to work with industrial partners in the production of windows to be used in field tests and a demonstration program. The overall program will be supported by BPA and DOE.

CHROMOGENIC MATERIALS RESEARCH

Optical switching materials or devices can be used to dynamically control transmission of solar radiation through a window by changing its optical properties in response to light, heat, or electrical field. Initial results of energy simulation studies of office buildings suggest that an automatically controlled switchable coating can provide substantial economic benefits by minimizing cooling and lighting energy use, reducing peak electrical demand and HVAC system size, and improving thermal and visual comfort. Thermochromic and photochromic systems may have less universal application than actively controlled electrochromic coatings, but may be simpler and cheaper to produce and perform equally well for specific building applications.

Electrochromic Materials

Electrochromism is exhibited by certain metal oxide and organic materials.[2] We are studying hydrated nickel oxide films and complete devices that include component layers such as polymer ion conductors. An anodic electrochromic material such as hydrated nickel oxide undergoes an intense color change after dual ionic and electronic extraction. An example of this reaction is: $Ni(OH)_2$ (transparent) <---> NiOOH, brown bronze+ H^++ e^-. This reversible reaction occurs at applied potentials below 1 Volt, and the material does not require a constant potential to remain colored.

Accomplishments During FY 1987

Our investigations have emphasized (A) developing a detailed understanding of the behavior of electrochromatic films to improve their operating properties, and (B) developing prototype electrochromic devices.

We have performed in-situ solar and FTIR spectroscopic studies on hydrated nickel oxide films in KOH electrolyte. These films were made by electrochemical deposition directly onto doped tin-oxide-coated glass substrates. We determined that in the bleached and colored states these films exhibit distinctive molecular vibrational states corresponding to $Ni(OH)_2$ and NiOOH, respectively. Also we determined the rate kinetics for specific conditions.[3]

In our device studies we developed a basic polymer electrolyte that conducts hydroxyl ions and used it to make the first prototype devices.[4] The devices are of the configuration: glass/SnO_2/$Ni(OH)_2$/polymer/SnO_2/glass. An example of the optical response of this device is shown in Figure 4. We also completed a study for the International Energy Agency (IEA) on the stability and durability of the most commonly known electrochromic devices.[5]

Planned Activities for FY 1988

The major objective in FY 88 will be fabrication of a complete optical switching device based on hydrated nickel oxide. We will continued to characterize and improve the polymer electrolyte and will develop better electrolyte deposition methods. We will expand our study of counter electrodes for ion storage and perform studies on optimizing and improving overall device properties. Our IEA studies

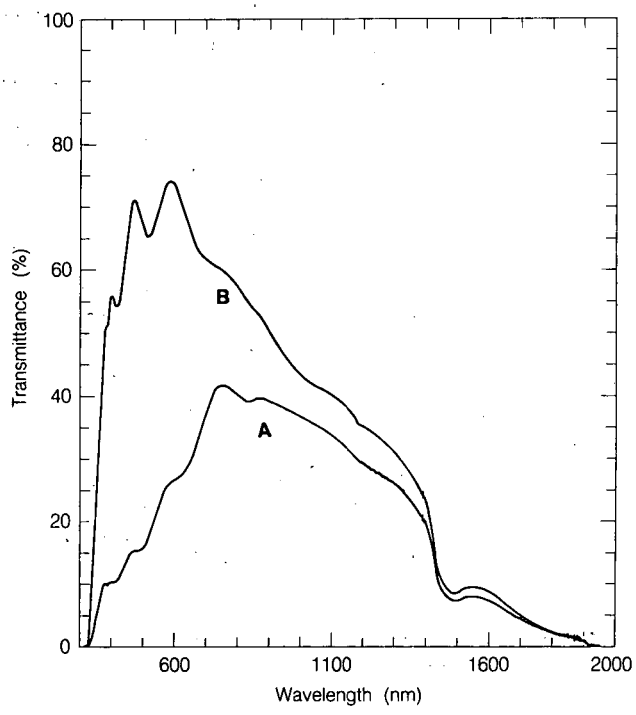

Figure 4. Normal solar spectral transmittance of the nickel oxide electrochromic device in colored (A) and bleached (B) states. The integrated solar and photopic transmittances are T_s (bleached) = 0.50, T_s (colored) = 0.23, T_p (bleached) = 0.70, and T_p (colored) = 0.23. (XBL 879-11135)

will investigate degradation and stability of generalized electrochromic devices.

Thermochromic Materials

Simpler thermochromic coatings that switch in response to heat or light may also be useful, particularly if these coatings can be fabricated and installed less expensively than more complex electrochromic coatings. A thermochromic material might, for example, be used in sun-belt residential windows.

Accomplishments During FY 1987

In FY 1987 we started work on a thermochromic vanadium oxide coating. Prior work by Honeywell suggested that VO_2 was a promising material, although its transition temperature was too high for use in buildings. Jorgenson successfully demonstrated that the transition temperature could be reduced by doping the oxide. We studied the optical and long-wave IR properties of the coating to determine its suitability for a combined low-E/thermochromic coating for windows in sun-belt residences. We concluded that the emittance was not low enough to provide useful insulating properties. The optical switching effects in the solar spectrum were disappointingly small for coatings that were thin enough to provide good light transmission in the clear state.

Planned Activities for FY 1988

There are several possible ways to increase the switching ranges. However, at this time we have decided not to pursue further research on this materials system.

MATERIALS FOR IMPROVED USE OF DAYLIGHT

Conventional methods of controlling daylight in buildings rely on architectural elements and shading devices. Greatly improved performance would result from materials or systems that could: (1) transmit maximum daylight with minimal cooling load impact (i.e., reject solar infrared radiation); (2) collect and distribute daylight beyond the perimeter zones in buildings; and (3) provide angular selectivity in accepting and redirecting incident light at the building envelope.

Light Guide Systems

Though daylighting can reduce electricity use and peak electric demand in buildings, its application is currently limited to work areas close to windows and skylights. Sufficient daylight falls on the exterior skin of a building to provide adequate illumination throughout any building—the technical challenge is to collect, transmit, and distribute the light where it is needed. We believe that light collection and transmission systems are the critical optical elements for successfully developing core daylighting systems. We are developing the system design concepts and performance data necessary to evaluate the economic feasibility of such systems.

Accomplishments During FY 1987

Previous simulation studies have shown that several types of solid and hollow light guides can transmit significant fractions of incident light. Performance is a function of materials, geometry, and incident sun conditions. Guide transmittance of greater than 50% is possible over a distance of 50 ft for a 2-ft-square guide. Optical measurements on a scale-model guide have corroborated these findings. We continued our mathematical studies of total optical system performance including the coupling between collector and guide optics. We established several baseline collector systems that could be coupled to each of several different guide systems.

Planned Activities for FY 1988

We will continue modeling studies to determine the overall performance of alternative optical system designs. We will complete a survey of several existing installations and will review the most promising optical systems from the perspective of costs and architectural integration. We will begin design studies for a core daylighting test facility that could be used by researchers or developers to test promising new systems.

ADVANCED GLAZINGS FOR AUTOMOBILES

Solar load control is an increasingly important problem to the auto and glass industries because styling trends and customer preference are dictating ever-increasing glass areas on car bodies. Also, the automobile industry and government have recently become concerned about auto air conditioners as a source of chlorofluorocarbon (CFC) in the atmosphere. Increased cooling loads associated with larger glazing areas demand larger air conditioners, which exacerbates the CFC problem. Our objective is to define the potential reductions in solar load and air conditioner size by using new high performance glazings.

Accomplishments During FY 1987

A series of parametric studies were compiled to document the effects of glazing properties on the cool-down characteristics of an auto air conditioning system (Figure 5). Using the computer program ESP,[6] we also analyzed interior air, dashboard, and seat surface temperatures as a function of exterior and interior surface absorptances, interior thermal mass, and air infiltration. We explored the possibility of cooperative studies between LBL and automobile and glass manufacturers and we established a working relationship with the Environmental Protection Agency, which is now formulating policy on the CFC problem.

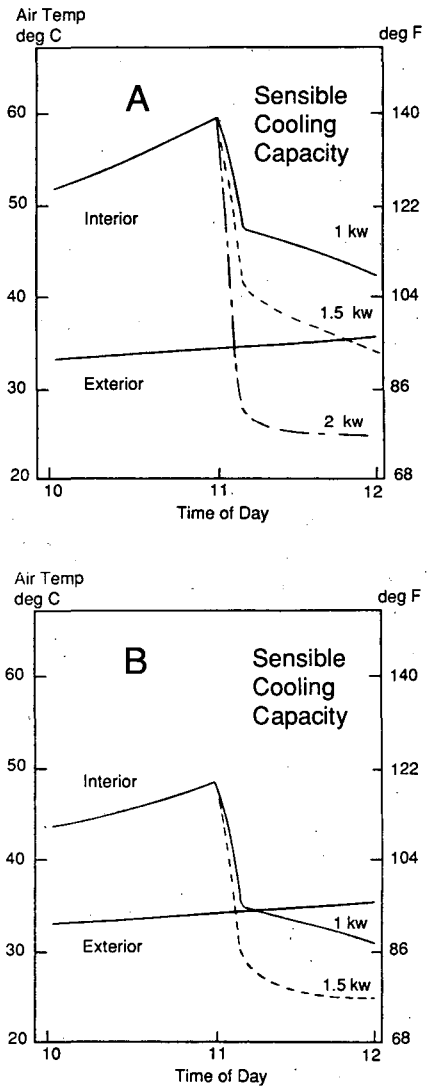

Figure 5. Interior air temperature in sports model as a function of time for varying air conditioner cooling capacity under static soak conditions. Air conditioner is turned on at 11 a.m. In A, glazing transmittance is 0.83; in B, 0.43 for front windshield and 0.23 for side and rear windows. (XBL 885-1480, XBL 885-1481)

Planned Activities for FY 1988

We plan combined analytical and experimental investigations of static-soak, cool-down, and city-driving conditions. We will revise the ESP simulation program to more accurately predict auto air conditioning performance. We will test the ESP program during our experimental measurements of air and surface temperatures, solar radiation, and air flow.

FENESTRATION PERFORMANCE

Research activities in this area are intended to characterize the performance of fenestration components and complete systems over the entire range of operating conditions in any climate or building type. The research will develop and refine experimental techniques and analytical models for accurately determining heat transfer and solar-optical properties of fenestration components and systems and will validate these models in field test facilities and occupied buildings. Many of the new algorithms and data sets are designed to be incorporated into hour-by-hour building energy simulation programs such as DOE-2.1. These data will not only improve the accuracy of our predictions but will also allow us to predict the performance of new fenestration systems and novel architectural designs. Our plan for developing and implementing these new analysis capabilities in energy simulation models is shown schematically in Figure 6.

THERMAL ANALYSIS

With the increased use of low-E coatings and gas fills, the number of possible window configurations is expanding rapidly. The continuing development of new products and their combinations necessitates an objective, accurate, easy-to-use calculational procedure to determine standard thermal properties. We developed and released WINDOW 2.0 in July 1986 to meet this need. It has been adopted by industry as a virtual de facto standard for window thermal calculations.

Accomplishments During FY 1987

During FY 1987 we completed work on WINDOW 3.0, which is to be publicly released in mid-1988. WINDOW 3.0 can now analyze certain gas mixtures, include the resistance of the glazing

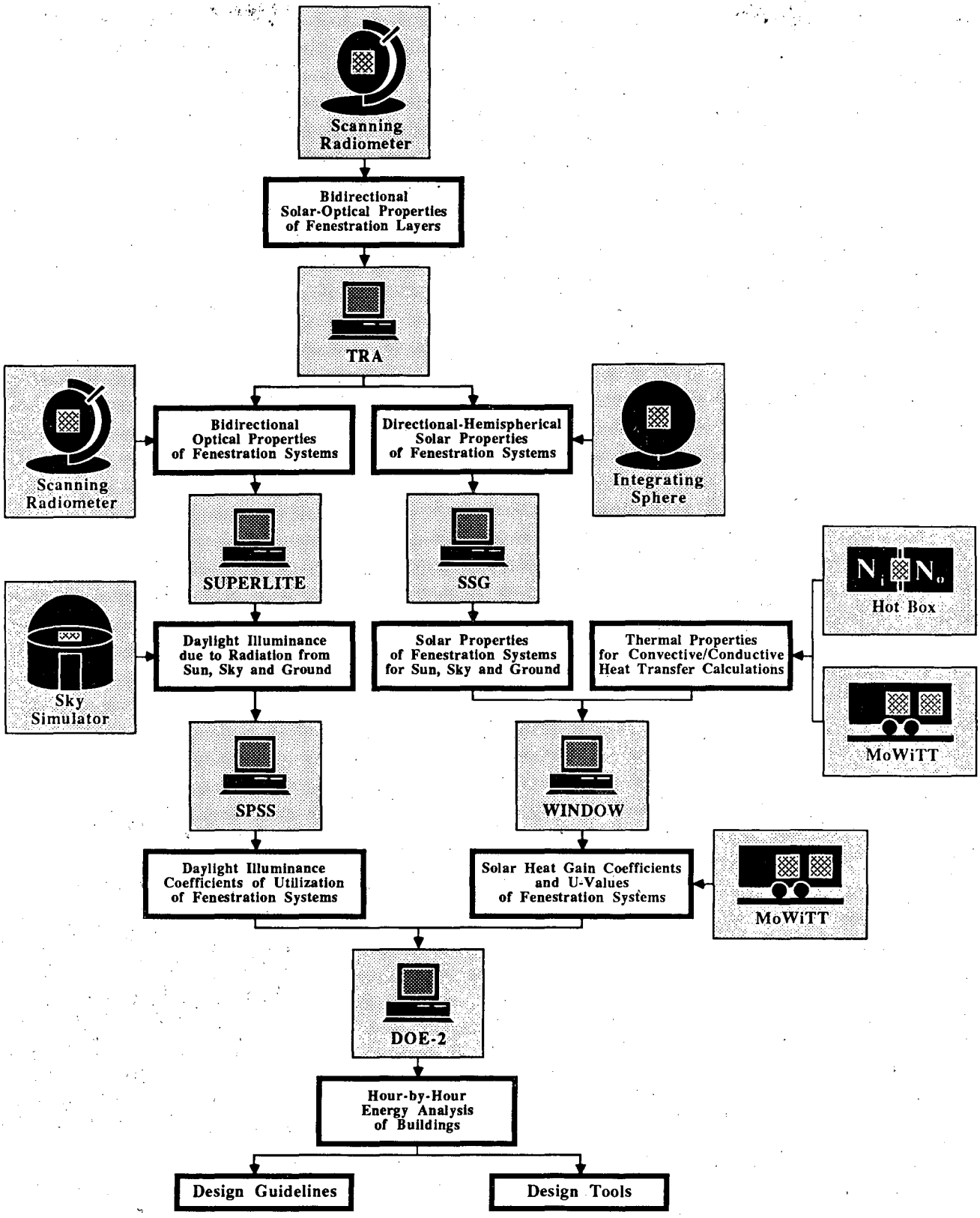

Figure 6. Schematic diagram of overall fenestration modeling capabilities under development including new measurement facilities, computer models, and intermediate calculated and measured results. Direct measurement of some intermediate calculated results provides a validation check. (XBL 885-1479)

material itself, use a multiband spectral-properties model, calculate two-dimensional edge and frame effects, and analyze nonvertical glazings. With the program's new interactive format, the user can make changes and see new results quickly. A new glass library allows the user to choose standard or user-input glass types and then quickly specify glazing choices by library number.

We distributed WINDOW 2.0 to approximately 200 users, including all major glass and window manufacturers. A major insulating glass sealant manufacturer has distributed over 500 copies of the program to interested recipients on their mailing list.

We also developed and distributed a spectral properties analysis program, SPECTRUM 1.1. This program calculates UV, visible, total solar, and IR average properties for a given wavelength-dependent glazing property. These results can then be used in WINDOW to calculate shading coefficient.

Planned Activities for FY 1988

During FY 1988 we will release WINDOW 3.0 to the public and continue to support and upgrade it in response to industry requests. The capability to analyze IR-absorbing gases will be added. The algorithms used in SPECTRUM 1.1 will be incorporated into a multilayer program compatible with WINDOW and will be distributed to interested users.

DAYLIGHT AND SOLAR HEAT GAIN STUDIES

Providing daylight to building interiors is one of fenestration's most important functions, both from an energy perspective and from an occupant's point of view. But the solar heat gain associated with daylight can be a benefit or cost, depending on circumstances. Analyzing the trade-offs to arrive at an optimum solution for simple glazings is difficult; for complex fenestration with sophisticated sun control systems it is virtually impossible with currently available tools. Our objective is to develop the experimental facilities and analysis models to accurately characterize the daylight and solar heat gain from fenestration systems of arbitrary complexity. We conduct a wide range of activities to establish the facilities, tools and data to address these problems.

Solar-Optical Properties of Complex Fenestration Systems

A quantitative understanding of the solar-optical properties of fenestration systems is essential to accurately predict their luminous and thermal performance for any sun, sky or ground conditions. "Luminous performance" refers to daylight illuminance and luminance levels used to determine electric lighting requirements and luminous comfort. "Thermal performance" refers to direct and diffuse solar heat gain levels used to determine heating/cooling requirements and thermal comfort.

The method that we are establishing (Figure 6) is based on treating fenestration systems as radiation sources of varying intensity distribution that can be calculated from their bidirectional solar-optical properties. The solar-optical properties of fenestration systems are determined from the bidirectional solar-optical properties of their component layers, using the computer program TRA (Transmittance/Reflectance/Absorptance). The bidirectional solar-optical properties of component layers are determined experimentally, using our scanning radiometer (Figure 7).

The output of TRA is used by the component programs SUPERLITE and SSG (Sun/Sky/Ground). SUPERLITE determines daylight illuminance and luminance coefficients. SSG determines direct (from the sun) and diffuse (from the sky and the ground) transmittance and absorptance (by component layer) coefficients for any sun, sky, and ground conditions.

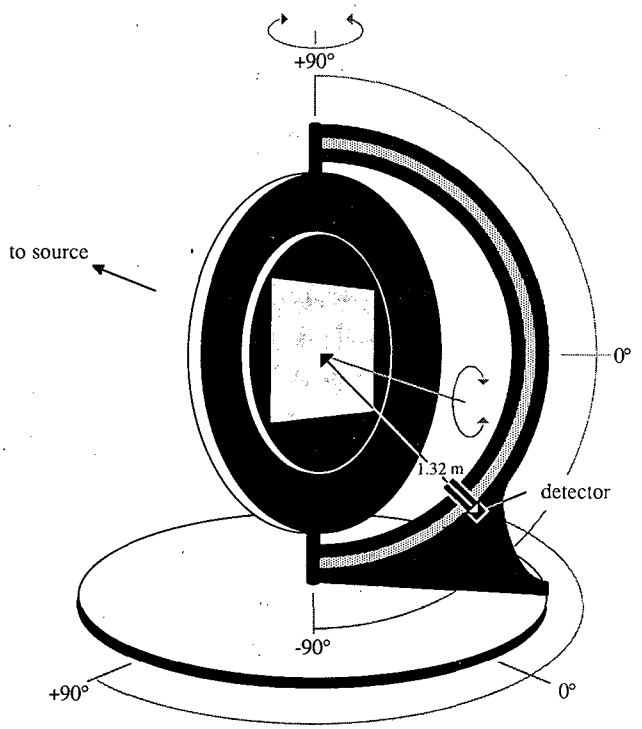

Figure 7. The scanning radiometer for measuring the bidirectional transmittance and reflectance of fenestration components and systems. (XBL 884-1472)

These direct and diffuse transmittance and absorptance coefficients are then used by the computer program WINDOW to determine solar heat gain coefficients.

Finally, the output of SUPERLITE and WINDOW is used by the computer program DOE-2.1 to determine hourly energy requirements for lighting, heating, and cooling and luminous and thermal comfort.

Accomplishments During FY 1987

Our work concentrated on the development of the scanning radiometer and the software for its operation, data acquisition and analysis. We also worked on the development of the computer programs TRA, SUPERLITE and SSG.

The scanning radiometer was fully automated and was used to determine the bidirectional optical properties of diffusing and slat-type shading systems (Figures 8 and 9). These measurements were used for identifying the limitations of our experimental techniques, as well as for validation of the computer program TRA. The scanning radiometer data analysis computer program and the computer program TRA were developed to operate on the same library of solar-optical properties of fenestration components and systems. A new version of SUPERLITE was developed to directly use the bidirectional transmittance coefficients produced by TRA.

The computer program SSG was developed for vertical and horizontal shading applications and was used with directional-hemispherical transmittance coefficients of venetian blinds (Figure 10) that were determined using our integrating sphere (Figure 11). SSG operates on the same solar-optical properties

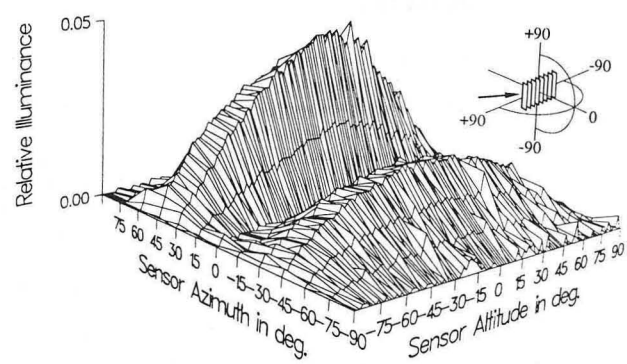

Figure 9. Transmitted distribution through a slat-type sample of 60-degree incident angle of incoming radiation on a plane normal to the slat direction. (XBL 884-1471)

library as TRA and accounts for the CIE standard overcast and clear sky luminance distributions and uniform luminance distribution for the ground.

Planned Activities for FY 1988

We plan to finalize our method for the simulation of luminous and thermal performance of fenestration systems. We will concentrate on installing the scanning radiometer in its new location in Building 70, and completing the final version of the operation and data acquisition/analysis hardware and software. Using scanning radiometer and integrating sphere measurements, we will validate our experimental procedures and the computer program TRA.

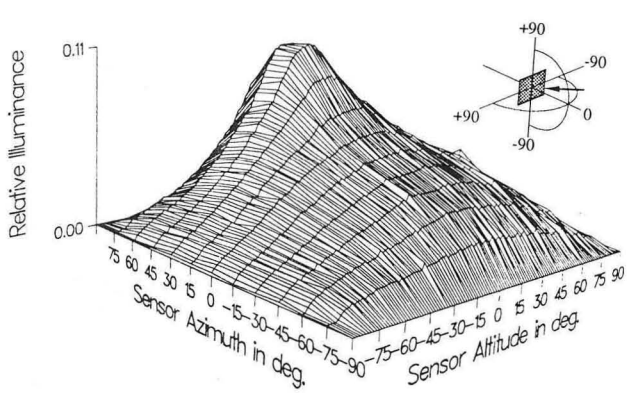

Figure 8. Reflected distribution by a diffusive sample for 45-degree incident angle of incoming radiation. (XBL 884-1470)

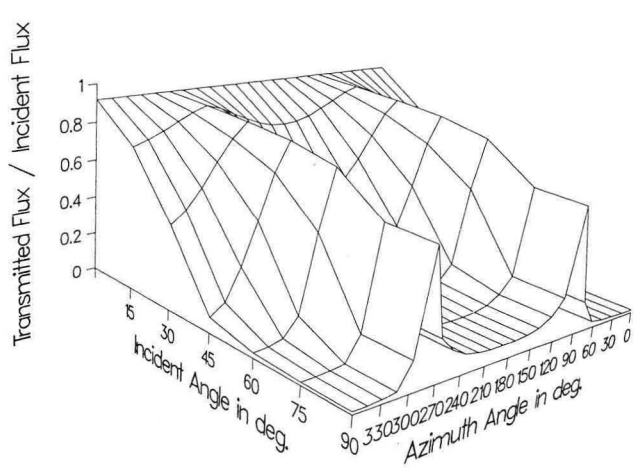

Figure 10. Directional-hemispherical transmittance of grey aluminum venetian blinds. (XBL 884-1473)

Figure 11. The integrating sphere for measuring the directional-hemispherical transmittance of fenestration components and systems. (CBB 837-6399)

DAYLIGHTING ANALYSIS

The prediction of lighting quantity and quality in the luminous environment is essential for energy-efficient lighting design. Over the years we have developed a range of daylighting design tools to expand our modeling capabilities and improve calculation accuracy. In the process, we have developed a state-of-the-art daylighting analysis model, SUPERLITE 1.0, which is widely used by researchers and to a lesser extent in lighting design. While continuing to expand SUPERLITE 1.0 to model more sophisticated daylighting systems such as complex fenestration systems, we enlarged the scope of our design tool development to include tools that can assist lighting designers in making qualitative assessments of luminous environments.

Accomplishments During FY 1987

We continued development of SUPERLITE and made progress toward modeling complex shading systems by incorporating measured bidirectional transmittance. We modified SUPERLITE to enable it to model optically complex fenestration systems with a bidirectional transmittance data set temporarily limited to 100 incoming and 100 transmitted light directions.

We collaborated with the ABACUS group, University of Strathclyde, Scotland, in developing an advanced lighting model to be incorporated into the three-dimensional color-rendering program DIM (Dynamic Illumination Model) that will not only produce numerical illumination levels but also display realistic images of a lighted space. The preliminary graphic images produced indicate a great potential for qualitative analysis of luminous environments (Figure 12).

Planned Activities for FY 1988

We will move beyond SUPERLITE's limitation on bidirectional transmittance data sets to enable us to model complex fenestration systems. We will begin validation of the new SUPERLITE model by comparing calculated results with data from scale model measurements. We will also develop the capability to display SUPERLITE output as three-dimensional shaded surfaces. We will also continue to collaborate with ABACUS to improve the new multichromatic lighting model.

Coefficient-of-Utilization Model for Energy Simulation Models

Computer models for building energy analysis must be able to predict the daylighting performance of the complex designs commonly used by innovative architects. The models should either internally calculate the daylight illumination or be supplied with data calculated by other illumination models or measured in scale models. The first approach, internal calculation of daylight illumination, is generally impractical for complex designs because of the significant computational cost and complexity required to obtain reasonably accurate answers. We are therefore developing a coefficient-of-utilization (CU)

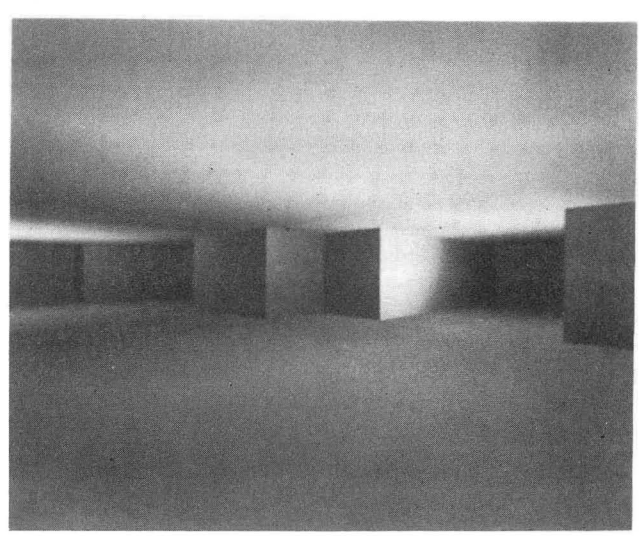

Figure 12. Image of a test space having surface luminance values calculated by DIM and plotted by a three-dimensional rendering program to display realistic images of the lighted space. (XBB 884-4095).

model that will be compatible with an hour-by-hour simulation model but still retain the flexibility and accuracy of more complex computational models.

Accomplishments During FY 1987

During FY 86 we developed the framework of our new daylight coefficient-of-utilization model; we identified seven indoor illuminance components based on the light sources (the sun, overcast sky, clear sky and ground) and the pathways (direct and indirect) to a location indoors. We also produced a new version of SUPERLITE 1.0 to be the primary source of indoor illuminance data.

Developing simple regression equations that can provide indoor daylight illuminance for a wide range of sun and sky conditions and for a variety of building configurations is a formidable task. During FY 1987 we focused on generating a CU equation for each illuminance component of a geometrically simple room. We generated seven principal forms of CU regression equations, aiming for expressions that are easily expandable and can handle the CU data from geometrically complex spaces in the future. The regression equations for direct components include variables relevant to window geometries, while those for reflected components include variables for room geometry and surface reflectances. Limited validation tests were also done.

Planned Activities for FY 1988

The improvements and detailed validation tests for the CU regression equations will be initiated. We will work with the DOE-2 group to add the new daylighting model to the DOE-2 program.

The Sky Simulator and Daylight Photometric Laboratory

A 24-ft-diameter hemispherical sky simulator (Figure 13) was designed and built on the University of California's Berkeley campus in 1979. In operation since 1980, it can simulate uniform, overcast, and clear-sky luminance distributions. Sky luminance distributions are reproduced on the underside of the hemisphere; light levels are then measured in a scale-model building at the center of the simulator. From these measurements we can accurately and reproducibly predict daylighting illuminance patterns in real buildings and thereby facilitate the design of energy-efficient buildings. The facility is used for research (Figure 14), for educational purposes, and on a limited basis by architects working on innovative daylighting designs.

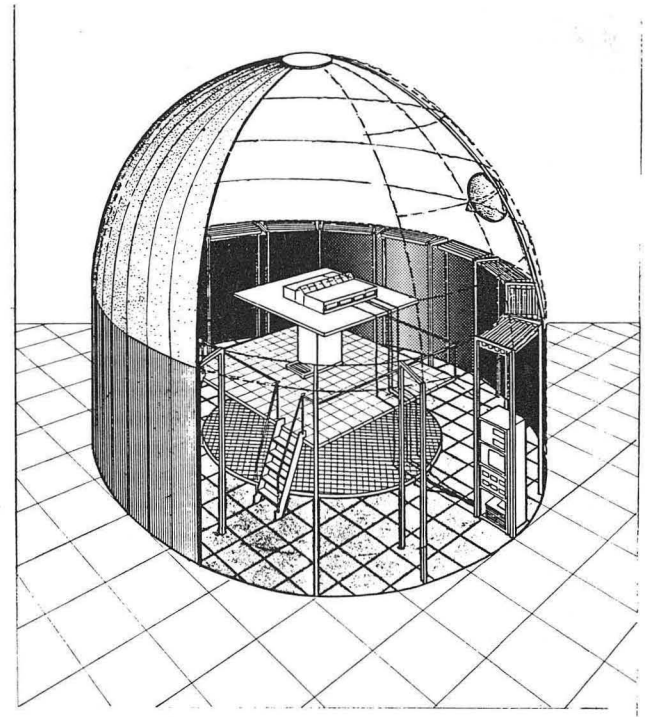

Figure 13. Schematic of 24-ft diameter sky simulator with model on platform. (XBL 8412-5328)

Daylight Availability Studies

Accurate daylight availability models are necessary for many design and energy analysis simulations. However, a widely accepted generalized model of availability in the U.S. has yet to be developed. We began work on this topic in 1978 and published three papers analyzing daylight availability data for San Francisco.[7-9] Analysis focused on the relationship of measured illuminance and irradiance to atmospheric parameters such as turbidity. New functional relationships were developed for an illuminance turbidity for visible radiation analogous to the conventional turbidity terms used with solar radiation and for zenith luminance as a function of turbidity. We found that our clear-sky luminance distribution data agree well with data from currently accepted European models.[10]

Our focus then shifted to developing a better understanding of the nature of partly cloudy skies. Although some progress was made using a sky luminance mapper, this activity was terminated due to budget limitations. We continue to collaborate on daylight availability with Florida Solar Energy Center (FSEC) where a new instrumentation package for detailed sky measurements is now in operation.

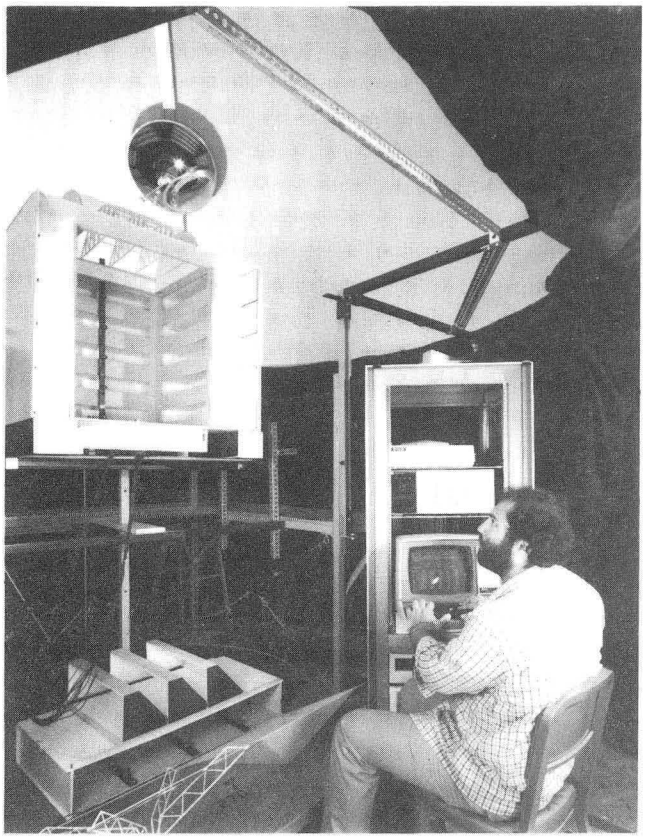

Figure 14. Interior of sky simulator showing reconfigurable scale model of a five-story atrium (with one side removed). (CBB 848-5926)

FIELD MEASUREMENT OF FENESTRATION THERMAL PERFORMANCE

We have known for some time that wintertime solar heat gain through south-facing windows in conventional buildings is a significant source of "free" energy. Subsequent calculations have indicated that it is technically possible, for any orientation in any U.S. climate, to optimize windows to the point that they become positive contributers to a building's energy needs.

This claim is not likely to be widely accepted without firm experimental verification. However, to measure the performance of highly optimized window systems in a realistic way is a formidable measurement task, requiring specialized non-steady-state calorimetry on a scale never before attempted.

To perform these measurements, a unique facility, the Mobile Window Thermal Test (MoWiTT) facility, was designed, built, and calibrated. In developing this facility it was necessary to solve the problem of doing calorimetry on a room-sized enclosure (which would normally require careful maintenance of constant equilibrium conditions) in the presence of the solar fluxes and changing outdoor temperatures that control the behavior of a fenestration system. We solved this problem with a large-area heat-flux sensor and a very sophisticated measurement of the heat extracted from the calorimeter by its cooling system. The MoWiTT, shown in Figure 15, began operation in 1986 at a field test site in Reno, Nevada.

Accomplishments During FY 1987

One of our first tasks was a study of newly commercialized low-emissivity insulating glazings. Though these glazings are offered by nearly every major U.S. glass and window supplier, there had been no convincing demonstration of their predicted energy savings in actual use, and the many products with different emissivities (hence, different U-values) had engendered considerable confusion in the marketplace.

A definitive study using the MoWiTT is ending this uncertainty. During 1986 we showed that these low-E insulated glazings show the expected improvement in U-value: a 35% reduction in nighttime heat loss. Further measurements of the net heat flow through the window demonstrated the effects of solar absorption in the low-E coating. Because of this absorption the overall effect of adding a low-E coating to double glazing is not simply the difference in nighttime heat loss: daytime solar heat gain is also

Figure 15. The MoWiTT facility at its field test site in Reno, Nevada. Two sealed insulating glass units are mounted in the two calorimeters. The portable building at left contains the computer that controls the facility and records data, including data from the on-site weather tower. (CBB 8611-10756)

reduced. The net effect of the fenestration on a building's energy balance depends on the extent to which the solar gain is beneficial or detrimental, and this depends on climate, orientation of the fenestration, and the building's heating and cooling demand and thermal storage capacity. Thus, knowledge of the true heat transfer through the window as a function of time is necessary to utilize the new window product in an optimal way.

During 1987 we extended these measurements to include cold winter conditions and other orientations. In Figure 16 the measured net heat flow through the fenestration over time shows the effect of U-value improvements for different orientations. Part (a) shows simultaneous measurements of low-E double glazing (points) and single glazing (solid curve) in a southern orientation (January 1987). Both fenestrations are large energy gainers during daytime; to the extent that this solar gain is useful, the lower transmission of the low-E tends to offset its nighttime advantage. The smaller daytime gains in the northern orientation (b) enhance the advantage of low-E (February 1987).

We studied the performance of a high-R, triple-glazed window incorporating two low-E coatings and a heavy gas fill. Figure 16 (c) shows that this window provides further improvement in a northern orientation. The shift in daytime net heat flow of the single glazing (solid curve) is a result of lower solar transmittance of the window and the higher daytime temperatures during these measurements (March 1987). The sharp daytime peaks in the single glazing curve are the result of transients in the measuring equipment and should be disregarded.

A systematic field study of the overall thermal performance of conventional glazing systems is also under way. Because window characteristics such as U-value are affected by ambient conditions, laboratory testing of window properties to predict the heating or cooling energy use attributable to the windows has been controversial. The impact of solar gain through windows adds further complications. Beginning with simple frameless windows and working toward progressively more complex systems, our study will test current methods (such as DOE-2) of calculating window performance in detail, and will delineate how useful simplified models as can be.

During 1987 we conducted extensive tests of windows with frames (a cooperative project with support from the Bonneville Power Administration). When completed, this study will demonstrate the importance of frame design and the accuracy of hot-box measurements for prediction of window thermal performance. Exploratory studies of air infiltration through windows were also begun.

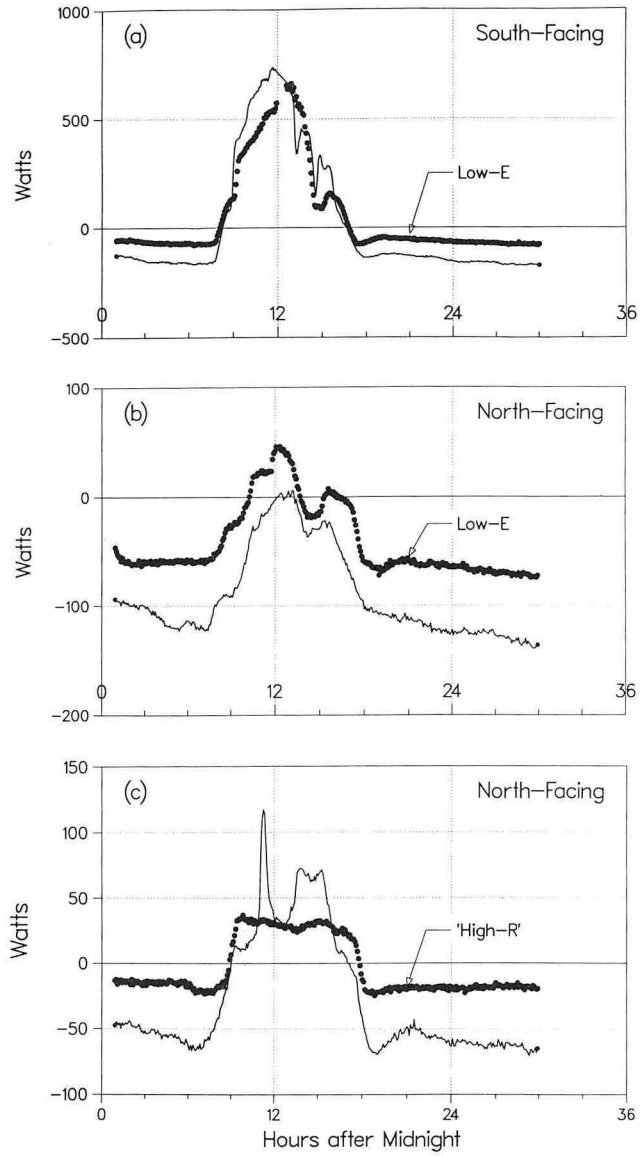

Figure 16. Measured net heat flow as a function of time. (a) Low-E (points) and single glazing (solid curve), south-facing. (b) The same pair of windows, north-facing. (c) High-R window (points) and single glazing (solid curve), north-facing. (XBL 884-1475)

Planned Activities for FY 1988

During FY 1988 we will further explore the relationship between thermal losses and solar gain with measurements of glazings of various transparencies and on managed fenestration systems. We will complete the study of windows with frames and begin a new study, in cooperation with ASHRAE, of solar heat gain through complex fenestrations including nonspecular shading devices. These and future measurements with the MoWiTT have the potential

for removing uncertainties about window performance that have slowed progress in energy conservation for a decade.

BUILDING APPLICATIONS AND DESIGN TOOLS

Research to develop new glazing materials and to better understand fenestration performance will provide real energy savings only if the technology is effectively applied in buildings. Using the technology requires that we have a detailed understanding of how a wide range of fenestration systems can be optimally used in different building types and climates, and that we pass this understanding, through design tools, to building design professionals.

SIMULATION STUDIES: NONRESIDENTIAL BUILDINGS

While most building energy simulation studies have focused on minimizing total energy consumption, other issues are equally important. Peak electrical demand affects both user costs and the utilities' required generating capacity. A complete study of the cost-effectiveness of fenestration systems, particularly those incorporating daylighting strategies, must include their impact on peak electrical demand as well as on energy savings. In addition, issues such as comfort and convenience affect the user acceptance and, consequently, the net energy efficiency of these systems. Our studies explore the interactions of these issues.

Accomplishments During FY 1987

During the past several years the effects of a wide range of glazing properties, window sizes, lighting loads, orientations, and climates on the energy performance of a prototypical office building have been simulated with DOE-2.1.[11, 12]

Initially we examined the impact of fenestration properties and daylighting strategies on office building energy performance and peak electrical demand. Lighting energy savings resulting from daylighting were examined for a range of fenestration properties and lighting control systems. Annual energy consumption of an office module was found to be sensitive to variations in U-value, shading coefficient, and visible transmittance, as well as glazing area, orientation, climate, and operating strategy. Sample results from our simulation studies are shown in Figure 17.

We conclude that, in almost all instances, it is possible to design a fenestration strategy that outperforms a solid insulating wall or roof, and that daylighting is almost always an essential component of energy savings. If the installed electric lighting power density is high, the energy savings potential is large. More efficient electric lighting systems reduce daylighting benefits.

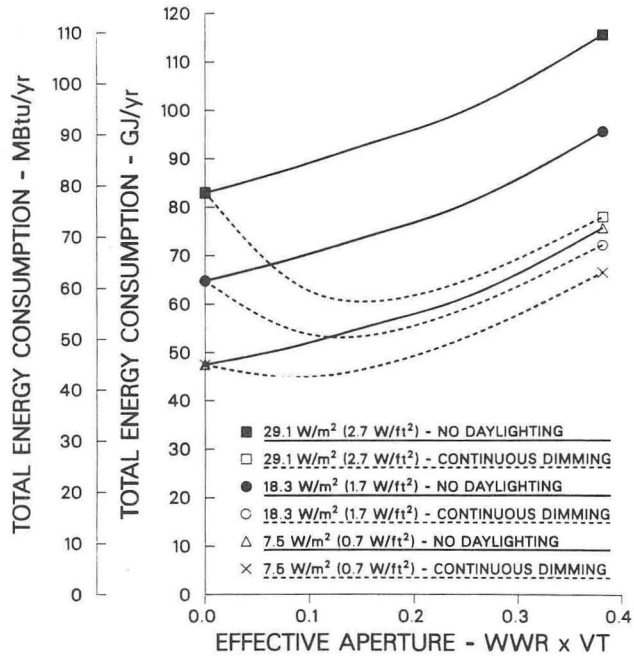

Figure 17. Annual energy consumption in the south zone of an office building in Madison, WI, as a function of window area. "Continuous dimming" indicates controlled reductions in electric lighting response to daylight; "no daylighting" indicates no dimming. (XBL 876-2796)

The net benefits of fenestration are highly dependent on the trade-offs between daylighting savings and cooling loads resulting from solar gains.[13] Visible transmittance properties, improved shading design, and window management will thus assume increasing importance for maximizing energy benefits from daylight. Our studies have demonstrated that the common assumption that daylighting is a "cooler" source of light than electric lighting is not necessarily true. In Figure 18 cooling loads for daylighting with several fenestration options are compared with cooling loads from electric lighting. We have developed and are refining a methodology[14] for comparing cooling loads imposed by daylight (or electric light) through the use of an index derived as a fraction of three parameters:

(1) the relative T_{vis} and SC of the glazing or shading system;
(2) the distribution of daylight within the space; and

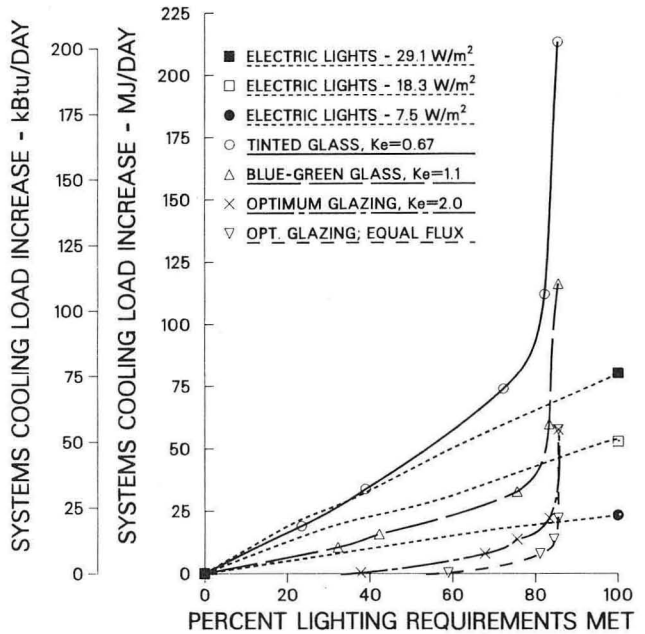

Figure 18. Increase in cooling requirements as a function of lighting strategy and glazing properties in a south zone on a clear March day. The "optimal glazing" has good selection properties (high K_e) and distributes the transmitted flux uniformly throughout the space. (XBL 884-1474)

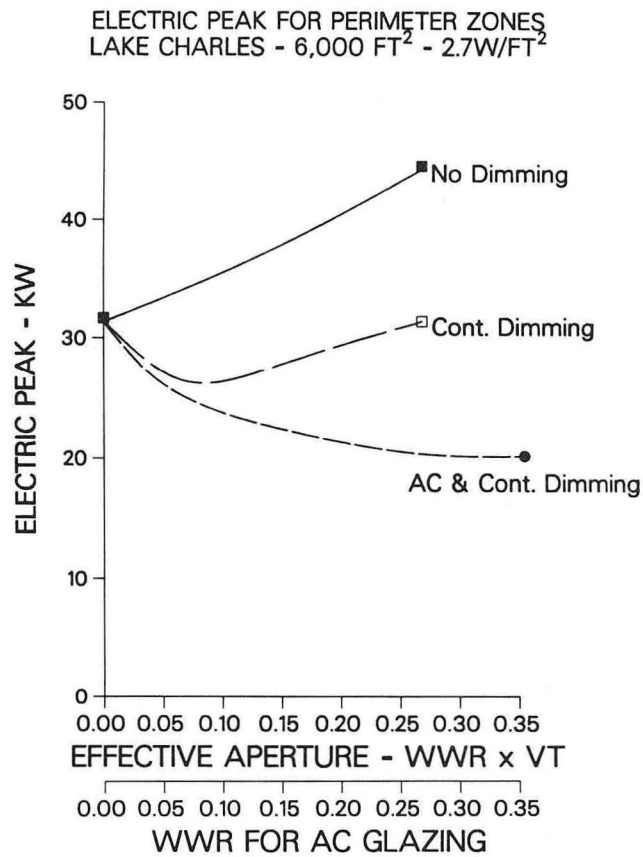

Figure 19. Results from DOE-2.1B energy simulations of a 6000-ft² office building in Lake Charles, LA, showing the effect of daylighting on peak electrical demand as a function of effective aperture. "AC" stands for a hypothetical glazing with transmittance actively controlled in response to solar gain level. (XBL 876-2802)

(3) the time-dependent absolute transmitted solar intensity.

We continued our general studies on the peak-shaving potential of daylighting with results that show—despite solar gains—daylighting can significantly reduce peak electrical demand during summer months. The critical trade-offs—between electric lighting reductions from daylighting and cooling load increases from solar gain—help determine the combination of window properties that minimize building peak loads. In Figure 19, annual peak electrical demand is shown for our prototypical building in Lake Charles, LA.

The most significant potential improvement in commercial building energy performance lies in the use of advanced glazing materials having dynamic optical properties and active response functions to control daylight and solar transmittance. Simulation results using these materials are shown in Figure 19 and compared to results with conventional glazing.

Skylights can also provide significant energy and cost benefits. Daylighting benefits are maximized with relatively small ratios of skylight effective apertures areas (0.01–0.04). Because skylights provide more uniform daylight distribution, the cooling load impact of daylighting may be less than with vertical fenestration. As effective aperture is increased beyond the optimum, cooling loads in most climates rise to adversely affect net annual energy performance.

A large number of DOE-2.1 runs for window and skylight studies have provided enough data for multiple regression techniques to develop analytical expressions of energy requirements as functions of glazing parameters; from these we may be able to develop a generalized expression to accommodate climate variables. The simple expressions correlate well with DOE-2 results and may become a design tool to assess energy and cost trade-offs among fenestration options. We have incorporated the regression equations developed in our skylight studies in a skylight design handbook sponsored by AIA, AAMA, and NFC,[15] and this procedure is the basis for the LRI fenestration performance indices described in the next section.

Planned Activities for FY 1988

New studies will examine the performance of more complex shading systems for which adequate solar optical data do not now exist. Optical properties of shading devices measured in our new laboratory facilities will be used in these studies. We will also continue to look at variations in window management strategies, issues of daylight luminous efficacy, advanced glazing materials, the effects of fenestration performance on HVAC, and the effects of various HVAC options on fenestration performance. The costs of fenestration design and daylighting as influenced by peak electrical demand, annual energy use, and chiller size will be examined.

FENESTRATION PERFORMANCE INDICES

We have completed the first phase of a two-part study to develop numerical indicators that can be used by architects, designers, builders, and others to determine the energy and comfort performance of fenestration systems[16]. Sponsored by the Lighting Research Institute, (with support from Electric Power Research Institute and New York State ERDA) the work was done in collaboration with the Florida Solar Energy Center. In Phase 1 we developed the basic methodology for determining the performance indicators in nonresidential buildings and tested the techniques for a few sample fenestration systems. In Phase 2, we will perform the measurement and analysis tasks required to construct a large data base of indices for most of the common generic fenestration systems. We also plan to develop a microcomputer tool to embody the project's results.

Accomplishments During FY 1987

We developed the concept and methodology for a fenestration performance design tool that will enable users to evaluate the fenestration systems of nonresidential buildings using a microcomputer. Performance indices for electric energy usage and peak demand, fuel usage, and thermal and visual comfort were established and a procedure proposed for the definition of an overall figure of merit. The figure of merit incorporates user-defined weighting factors that assign relative weights to each performance index. Figure 20 shows sample figures of merit for evenly weighted performance indices for four glazing types. We developed a prototype computer design tool so that potential users can evaluate the methodology and offer recommendations for improving the final tool in Phase 2.

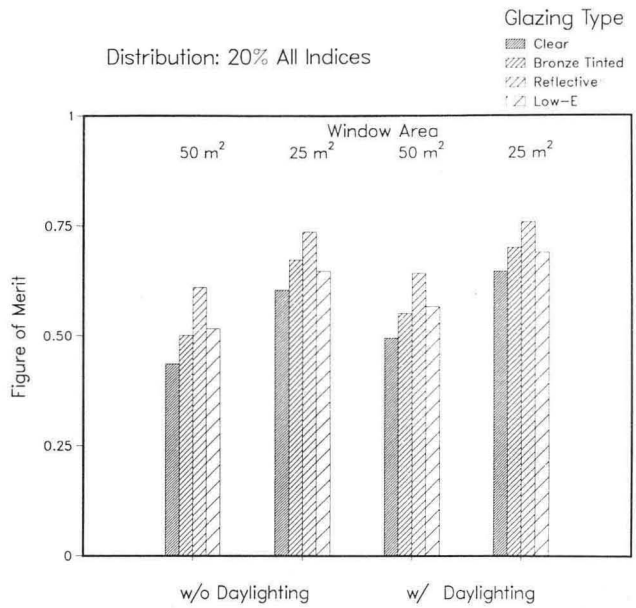

Figure 20. The figure of merit compares the performance of fenestration systems. Here the five performance indices are equally weighted (20% each). Results are shown for four glazing types and two window sizes, with and without lighting controls and daylighting. (XBL 884-1476)

Planned Activities for FY 1988

We will begin Phase 2 during FY 1988. Performance data will be calculated and a computerized data base constructed for conventional fenestration systems and complex operable shading systems. The primary Phase 2 product will be a microcomputer tool to access and process the fenestration data base and to apply user-defined weighting functions. The specific form and capabilities of the final tool will be based on extensive consulation with the project sponsors and feedback from professional user groups.

SIMULATION STUDIES: RESIDENTIAL BUILDINGS

The growing number of new window technologies in the residential sector make window selection a difficult task. Over the last few years we developed analytical techniques to predict window performance for a wide range of technology options and climates.[17] We have developed a regression analysis method to translate an energy use data base into algebraic expressions to directly calculate which window properties will optimize energy use or other values. Our analysis efforts are beginning to show potential for developing powerful new tools for determining residential fenestration performance.

Accomplishments During FY 1987

We continued our analytical studies to simplify the procedures for predicting the energy effects of windows in residences. We concentrated on determining the relationship between different residential prototypes so that in the future we can significantly reduce the number of required computer simulations. We continued studying our regression expressions to better understand the component load and incremental costs associated with windows. Extensive data on low-E window performance were generated for Madison, WI, Lake Charles, LA, and Phoenix, AZ (Figure 21).

Reliable and accurate data on energy performance are needed by builders in a form that is easily accessible and useful in building design. Working with representatives of the residential building industry, we began efforts to make our technical information available to designers by translating it into accessible formats.

Planned Activities for FY 1988

Our objective is to develop handbooks, charts, nomographs, and computer software to help builders and suppliers assess window strategies. The immediate goal in FY 1988 is to develop a series of informative "design notes" for builders and to create a prototype residential fenestration design tool to stimulate building industry interest in collaborative development of a comprehensive tool.

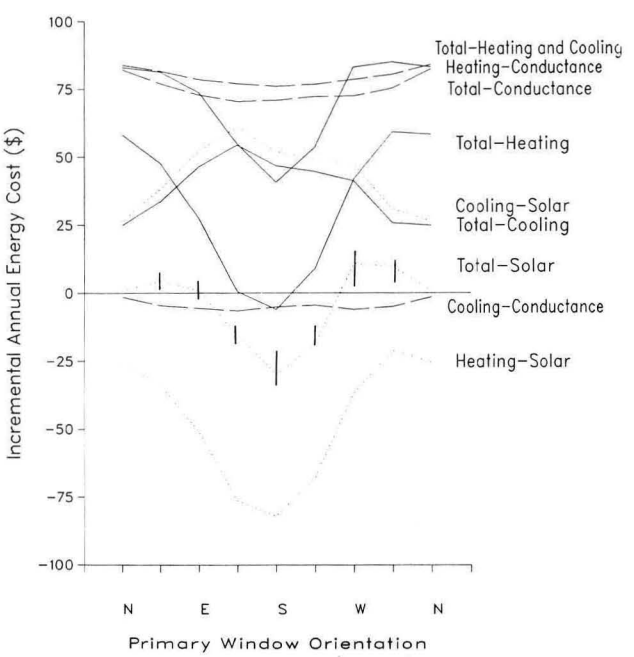

Figure 21. Incremental annual energy cost components for varying orientation of a double-pane window with low-E coating with an area of 18.39 m^2, U-value of 1.94 W/m^2C, and shading coefficient of 0.73, in Madison, WI. Positive values represent heating costs, negative values heating savings. (XBL 885-1478)

DESIGN TOOLS AND TECHNOLOGY TRANSFER

To influence energy consumption trends in the United States, it is critical to communicate our results to other researchers and professionals. We use a variety of media to reach a widely varied audience: other research and development groups, educational institutions, and professional and industrial societies. We have developed improved daylight analysis and design tools and handbooks, carried out design assistance studies, and sponsored workshops and meetings with manufacturing and design firms and public utilities.

Technology Transfer

We continually communicate research results to design professionals and industry through conferences, workshops and seminars.

Daylighting Conferences. At the conclusion of the 1986 International Daylighting Conference, we assisted in promoting the conference's general proceedings[18] to professional and industrial societies and educational institutions. The refereed technical proceedings will be published in 1988.[19]

Daylighting Network of North America. After several years of organizational growing pains the Daylighting Network of North America (DNNA) has established an active membership of 35 universities with research and instructional interests in daylighting. The DNNA has expanded the avenues for transferring daylighting research results to professionals, educators, and students.

In FY 1987 faculty and students from several DNNA centers worked at LBL on daylighting projects. We plan to continue these informal exchanges in FY 1988. LBL also supported an electronic network of eight authors from different universities jointly writing a handbook, *Simulating Daylight with Architectural Models.*[20]

The Network makes a concerted effort to plan and implement professional educational and design assistance programs. One successful vehicle has been the *DNNA News*,[21] currently published at the University of Michigan. SUPERLITE 1.0 and DOE 2.1B and C continue to be disseminated to faculty

and practitioners by one of the regional centers. Of special significance is a three-year major research and education effort at the University of Minnesota DNNA Center. Faculty will be developing professional workshop curriculum, computer course demonstrations, and daylighting information data bases for students and building professionals in the state, using many daylighting tools and data bases developed at LBL.

The Network will continue to distribute design software and promote joint research projects. Establishing a sabbatical-timed program for visiting researchers at LBL will be a priority.

Design Tools

The Windows and Daylighting Group and subcontractors develop and distribute daylighting design tools to industry and educational institutions. Private-sector software firms continue to introduce new design tools for daylighting, but evaluation and comparison are difficult. There is a need: (1) for a comparative matrix identifying the capabilities of existing tools, and (2) for photometric data and evaluation procedures to compare these tools.

Accomplishments During FY 1987

We continued distribution of the Daylighting Design Tool Survey,[22] SUPERLITE, Daylighting Nomographs and other tools and data.

Skylight Handbook/Design Guidelines. The *Skylight Handbook,*[15] based on technical research done by LBL, was completed and published by the Skylight and Space Enclosure Division of the American Architectural Manufacturers Association (AAMA), and distributed to building professionals. The handbook's energy design data worksheets will be converted to a microcomputer program during the coming year. The *Skylight Handbook* is expected to serve as a model for joint development of handbooks and design guides with other public and private professional organizations.

Advanced Design Tool. Our long-term interest is in the development of the next generation of sophisticated hardware and software design tools. The Advanced Envelope Design Tool (AEDT) development has moved on several levels over the past year. The computer data base of hardware and software continues to track market trends. We have formed professional liaisons with major architectural firms, software manufacturers, and building organizations for the purpose of developing joint activities. Believing imaging technology to be a key to any future design tool, we have explored CD-ROM technology for possible use in the AEDT. We also continued investigations of knowledge-based systems and advanced simulation models at a low level.

Planned Activities for FY 1988

We plan to form a Berkeley working group of research projects at the University of California and LBL. With combined resources and expertise, the development of a prototype interactive microcomputer-based tool to illustrate the potential of the AEDT could be realized.

We expect to integrate our interest in the Advanced Envelope Design Tool with a broader DOE-sponsored effort on advanced tools for whole-building design.

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Lighting Systems Research*

S.M. Berman, R.R. Verderber, R.D. Clear, D.D. Hollister, D.J. Levy, O.C. Morse, F.M. Rubinstein, M.J. Siminovitch, G.J. Ward, and R. Whiteman

We estimate that 50 percent of the electrical energy consumed by lighting, or about 12 percent of total national electrical energy sales, could be saved by gradually replacing existing lighting with energy-efficient lighting. This would amount to a yearly savings of some 220 billion kilowatt-hours of electricity.

The objective of the Department of Energy's National Lighting Program is to assist the lighting community (manufacturers, designers, and users) in achieving a more efficient lighting economy. The program carried out at Lawrence Berkeley Laboratory (LBL) represents a unique partnership between a national laboratory-university complex and industry, facilitating technical advances, strengthening industry capabilities, and providing designers and the public with needed information.

To implement its objectives, the Lighting Program's efforts are divided into three major categories: advanced light sources, building applications, and impacts on human productivity and health.

The advanced light sources component undertakes research and development projects that are both long-range and high-risk, leading to more efficient sources of light. These are projects in which the lighting industry has an interest, but which it does not pursue on its own, and from which significant benefits could accrue to both the public and industry. These efforts involve the disciplines of physics, chemistry, and electrical engineering.

The building applications component undertakes research on the electromagnetic compatibility of high-frequency lighting with building functions, including machinery, computers, and other electrical and electronic systems; the interaction of lighting with building energy systems; and the use of lighting controls and fixtures to optimize lighting benefits. These efforts combine the disciplines of engineering, architecture, and lighting design.

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The impacts component examines relationships between humans and lighting, looking to ensure that energy-efficient technologies contribute positively to human productivity and health. These efforts are interdisciplinary, involving engineering, optometry, physiological optics, and medicine.

Since its inception in 1976, the LBL Lighting Program has produced more than 124 reports and publications. These reports are available to the public and document research on subjects such as solid-state ballasts, operation of gas-discharge lamps at high-frequency, isotopically enriched fluorescent lamps, energy-efficient fixtures, lighting control systems, and visibility and human productivity. In addition to its research activities, the internationally recognized interdisciplinary staff is involved in a variety of professional, technical, and governmental activities.

The Lighting Program combines the facilities and staff of LBL with those of the University of California College of Environmental Design and School of Optometry, both on the Berkeley campus, and the School of Medicine in San Francisco (UCSF). Because the research is directed at both enhancing the capabilities and long-term viability of the lighting industry, and providing the design profession and the general public with needed information, the program is unique in the United States and the world.

Described below are highlights of the accomplishments realized in FY 1987 and activities planned for FY 1988 by each of our three major efforts: advanced light sources, building applications, and health impacts. Publications and conference presentations from the past year may be found in the publications list at the end of this chapter.

ADVANCED LIGHT SOURCES

The advanced light sources effort promotes new lamp technology and light source development. To see what can be accomplished in this area, consider that the most efficacious four-foot fluorescent lamp, operated at high frequency (20 kHz), has a luminous efficacy of approximately 100 lumens of light output per watt of electrical power input. Although this is more than five times as efficient as an incandescent lamp, still greater efficacies are possible. White light can, theoretically, be produced at almost 350 lumens per watt. The advanced lamp technology program is developing the engineering science that will help us achieve a target efficacy of 200 lumens per watt within the next few years. Table 1 lists the series of technical improvements that are proposed to reach that goal.

Eliminating three significant loss mechanisms—self-absorption of ultraviolet (UV) radiation, electrical losses, and energy loss in lamp phosphors—in fluorescent lamps will improve their efficiency. In the first case we would like to reduce self-absorption of UV radiation, a process that occurs within the lamp plasma before the radiation strikes the phosphor-covered inner wall (the phosphor converts UV radiation into visible light). If, we decrease UV self-absorption, we increase the amount of UV radiation available to be converted into light, and therefore increase the lamp's light output.

In the second case, energy losses associated with electrodes can be eliminated by exciting the lamp plasma at radio frequencies (RF). The problem is to find an efficient method for coupling the RF energy into the lamp without causing new losses.

In the third case, we would like to develop a more efficient phosphor matrix that will convert one energetic UV photon into two visible photons. Reductions in self-absorption and electrode losses could provide a significant improvement, and a two-photon phosphor could double lamp efficacy.

LBL is studying several ways of reducing UV self-absorption. The first method is altering the isotopic composition of mercury. In its natural state mercury has seven stable isotopes, each with slightly different resonance UV emission spectra. Altering the naturally occurring isotopic composition can provide more escape channels for the resonance radiation, thereby reducing the probability of quenching collisions and increasing the amount of UV radiation reaching the phosphor. The most promising possibility is isotope alteration-enrichment with ^{196}Hg, which is being pursued in a joint effort by LBL and GTE Lighting. Should isotopic alterations prove economical, modified lamps would enter the market quickly. Lamps would simply be loaded with isotopically enriched rather than natural mercury, with other lamp manufacturing processes remaining the same.

Another method of reducing UV self-absorption was recently discovered at LBL based on the application of a d.c. magnetic field having a direction parallel to the main current. Axial magnetic field strengths of about 600 gauss can increase light emission by about six percent. LBL and major firms in the lamp industry are studying practical ways to apply this technique.

A highly promising mechanism developed at LBL uses a plasma coupling principle that eliminates the need for electrodes, it allows for lamp plasma excitation to occur primarily near the inner lamp wall and thereby, reduces both the electrode losses and the likelihood of entrapment loss. This surface wave mode of operation occurs at high frequencies, in the radio frequency (RF) range between 100 and 500 MHz, permitting efficient lamp excitation without electrodes. The surface wave lamp shows approximately 40 percent increased energy efficacy over normal fluorescents, operates without starting circuits, and should be very long lasting because of the absence of electrodes.

Reducing the effects of energy loss in the phosphors requires altering a lamp's phosphor material. The materials used today convert each UV photon into, at most, one visible photon. Improving this conversion rate would increase the efficacy of low-pressure discharge lamps. Although a UV photon has sufficient energy to permit the cascade conversion of the UV photon into two visible photons, this process must occur quickly to prevent heat-producing collisions. The intermediate level in the cascade must be tuned carefully, ensuring that both emitted photons are in the visible spectrum. LBL is examining the possibilities of a program in phosphor chemistry designed to discover whether the two-photon phosphor is feasible. The lamp industry, long aware of the complexity of this problem along with the extensive research required to provide solutions, is extremely interested in a cooperative effort.

If these research projects at LBL come to technological and commercial fruition, future fluorescent lamps should operate at high frequency and be isotopically enriched, magnetically loaded, and coated with a two-photon phosphor. Such lamps would have an efficacy of more than 200 lumens per watt, doubling the efficiency of today's best fluorescent lamps.

Other lighting technology research concentrates on high-intensity discharge (HID) lamps, which could be made both more efficient and dimmable if operated without electrodes. High-frequency operation is required to excite the lamp plasma in an electrodeless mode; it may also permit lamps to function with just one or two metal halides and no mercury or sodium. Electrodeless operation would also enable us to use compounds that have desirable light output and color, but that are excluded today because they would harm electrodes. Finally, an electrodeless lamp that could be dimmed without observable spectral changes and that could provide instant restrike could be used in many new ways improving energy efficiency and is therefore attractive to lighting designers. Table 1 summarizes our goals.

To address the lack of data on the plasma discharges, a program on plasma diagnostics has

Table 1. Targets of opportunity in lighting technology.

Technology	Comment	Total efficacy (lm/W)	Year entering market
Fluorescent lamps			
High-frequency operation		90	1980
Narrow-band phosphors		100	1983
Isotopically enriched	LBL/DOE	110	1988
Magnetically loaded	technical	120	1990
Two-photon phosphor	initiatives	180	1995
Gigahertz/electrodeless		230	1995
HID Lamps			
Today with (high-freq. ballast)			
400-W high-pressure sodium	(CRI-25)	100	1984
400-W metal halide	(CRI-66)	80	1984
400-W mercury	vapor	50	1984
Electrodeless/high/freq.			
1000-W lamps	10-15% improvement		1989
Low-W lamps	30% improvement		1989
New gases	20-25% improvement		1990
Color-constant/dimmable	20-25% improvement		1993

been initiated. It will measure a number of characteristics of both optically thin and thick plasmas (see Fig. 1).

Accomplishments During FY 1987

Mercury Isotope Separation and Enrichment

Continued progress has been made in assessing the feasibility of photochemical separation of natural mercury to produce mercury enriched in the isotope mass 196Hg. Three significant accomplishments achieved during FY 1987 are discussed below.

Basic to the photochemical process is the establishment of a high flux source of nearly pure 196Hg photons. This source is a centrally located quartz lamp that is filled with as pure a charge of 196Hg as possible. However the initial sample of mercury is not 100 percent pure and because the 196Hg hyperfine resonance line has some overlap with other isotopes, added frequency filtration is required to assure a pure product. As part of the separation system, frequency filtration has been successfully added that achieves the desired high photon flux with good isotopic selection.

The second accomplishment was measuring the overall transmission of the inner annulus wall of the reactor chamber, as a function of time and material deposition rate, to study the possibility of reducing in the incoming photon flux.

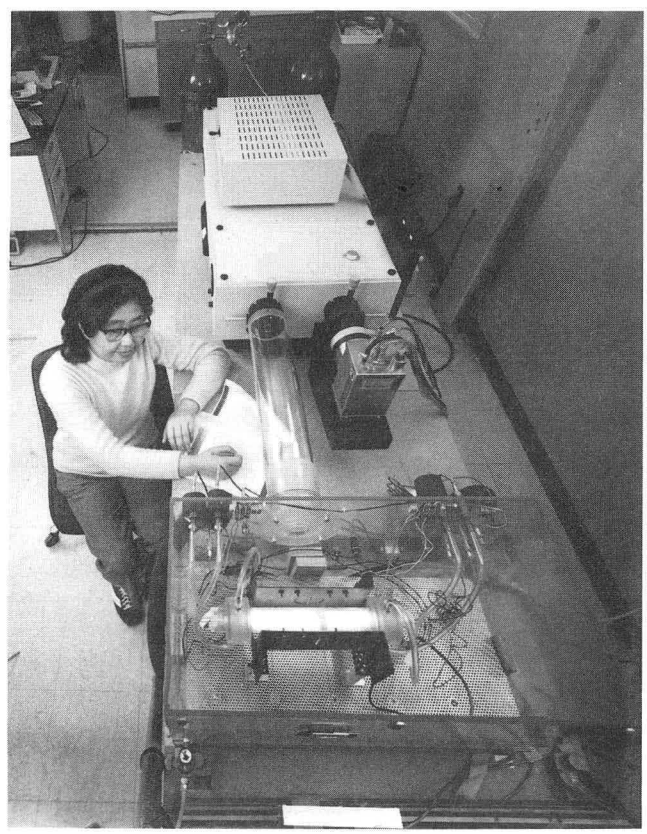

Figure 1. A test fluorescent quartz lamp loaded with a particular admixture of mercury isotope is examined spectroscopically at the UV resonance line. (CBB 870-9874)

The third accomplishment was the development of a new practical means of removing the product separated isotope in a continuous, rather than batch, process.

Magnetic Enhancement

The luminous efficacy of a 7-inch fluorescent lamp immersed in a nearly uniform axial magnetic field has been examined. We made provisions to isolate the electrode power loss from the total observed lamp dissipation in order to assure that the actual positive column luminous efficacy was indeed being determined. Data were taken for cold spot temperatures in the range (30 T < 48) and applied magnetic fields in the range (0 B 965 gauss). We found that the luminous efficacy of the positive column showed a maximum, with a cold spot temperature of 40.7° C and an applied magnetic field of 845 gauss. These data represent a 6.14 percent increase over the positive column luminous efficacy in the absence of an applied axial magnetic field. All measurements were made with constant arc current.

We observed that the total dissipation of the lamp under test increased with increases of applied axial magnetic field. Evaluation of the electrode power losses indicated that most, if not all, of the increased power requirement was dissipated at the electrodes, while the positive column dissipation remained approximately constant for all values of magnetic field studied herein.

The establishment of the size of the magnetic effect completes our investigation. Any further effects would be directed toward developments of viable methods of bringing a magnetic field into a lamp's environment.

Surface Wave Lamp (SWL)

Many detailed technical problems have been solved during FY 1987. In particular the thermal control system, the optical detection system, and the RF detection system have all been upgraded. We constructed a modular RF cage a modular RF cage to handle tubes from seven inches to four feet in length. The cage's wire geometry allows most of the light emanating from the lamp to be visible.

The surface wave lamp demonstration for display in the U.S. Senate building has been completed. We overcame a number of technical problems so that a non-technical person can operate the demonstration system and show the surface wave lamp's 40 percent improvement, in efficiency over an a.c. fluorescent lamp.

Our development of a special facility for high-intensity operation of a surface wave lamp has continued on schedule during the past year, including completion of the RF shielding, the optical collimator system, and the RF power measurement system. In addition, the high intensity launcher has been designed and should be fabricated during FY 1988.

End Fall Diagnostics

Further diagnosis of the end fall power losses by the movable cathode technique has been delayed because the test lamp was not fabricated according to specifications. A new test lamp is expected in early FY 1988. Using the imperfectly fabricated lamp, we compared measurements of voltage by moving the cathode with and untested current variation method yielding consistent but somewhat limited results. Tests with the new lamp are expected to clear up the present uncertainties.

Planned Activities for FY 1988

Mercury Isotope Separation and Enrichment

We will begin designing and constructing the next reactor of increased size and capacity, which will be capable of producing several grams of enriched mercury per day. We will use knowledge gained from using the smaller reactors to help us design the new one. Access, geometrical configuration, as well necessary spectrographic instruments will be taken into account in the new design so we will be able to measure the emission and absorption line profiles of the ^{196}Hg under conditions of variable reactant pressures and temperatures. Thus, the new design will permit thermodynamic sensitivity studies on the ^{196}Hg production as it depends on the HCl, Hg, and rare gas conditions. The new design will also permit measurement in-situ of performance and allow continuous monitoring of the processes. These efforts should lead to the production of enough enriched mercury that we can evaluate high-speed production of fluorescent lamps with the enriched product.

Electrodeless High Intensity Discharge (HID) Lamp

This project will start during FY 1988; first we will set up an induction system for operating experimental low wattage HID lamps at frequencies of 6.87, 13.56, 27.12, and 40.68 MHz. We will be able to introduce new gas fills to compare the new experimental lamps with existing low wattage electroded lamps. Special care will be taken to assure the accuracy of power measurements at these high frequencies; these measurements have been a major prob-

lem. Previous work by General Electric for LBL, has shown that bromide and chloride salts can produce good color and high efficacy in electrodeless HID lamps at high powers (1000 watts). After geometrical configuration permitting low power operation have been established, experimentation will begin on the applicability of the new gases in these low power configurations.

Surface Wave Diagnostics

The radial distribution of electrons (or ions) and excited mercury atoms is expected to be more skewed toward the lamp wall in the surface wave lamp than in the standard 60 Hz a.c. fluorescent lamp. General Electric Corporate Research and Development has a laser diagnostics which can measure mercury excited state radial distributions by the method of induced fluorescence in the a.c. lamp. We expect to negotiate a subcontract with GE asking them to extend their laser diagnostics capability to the surface wave lamp.

Surface Wave Lamp (SWL)

Optimization of the SWL parameters such as mercury and argon pressures, glass thickness, as well as operating frequencies is fundamental to establishing lamp efficacy. These measurements require several hundred test lamps, all of which will be fabricated by an outside vendor because we currently cannot produce them in house. Toward the end of FY 1988, subsequent to the addition of more laboratory space, a new lamp fabrication facility will be designed and installed as part of the lighting laboratory. In addition, when the optimum frequency characteristics have been established, an RFP will be developed to interest the electronics industry in a low-power high-frequency power supply.

BUILDING APPLICATIONS

Real energy savings depend on the transfer to the lighting community of energy-efficient technologies and strategies. The building applications activities aim to assess and, develop energy-efficient lighting technologies and combine their technical performance characteristics to model energy-efficient and cost-effective lighting geometries and controls. Our analysis uses knowledge of the relationship between visual performance and physical aspects of lighting, such as illumination level, distribution, contrast, and glare. As part of this effort, a computer program has been developed that provides accurate simulations of illuminated spaces with their contents. The simulated scenes are visibly indistinguishable from real photographs; using them, we can model effects of changes in the illumination systems. Validation of luminance values produced by these simulations requires physical measurements of luminances in complex environments. Therefore, the project uses a number of novel techniques for luminance mapping of interior environments with complex objects to obtain actual luminance values. The technology development component of this program examines engineering approaches to reducing light losses associated with conventional lighting fixtures. The conclusion of these efforts will be a combination of lighting systems technologies and analysis with a visual simulation of the proposed application representing the most compelling tool for promoting the implementation of energy efficient lighting. (see Fig. 2).

Accomplishments During FY 1987

Advanced Lighting Design

We selected a workspace for the Lumen-Micro computer program, which includes input from a variety of luminances and control systems. The program is then augmented and used to calculate the two principal metrics for assessing the value of a lighting environment: the average relative visual performance (RVP), and the visual comfort probability (VCP), a measure of glare present in the system design. These metrics, along with lighting energy economics, are the basis for a cost benefit analysis that can incorporate the engineering parameters of lighting systems.

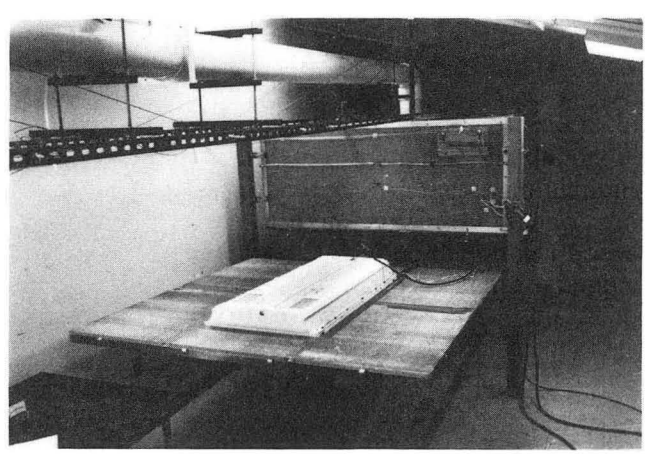

Figure 2. The testing facility for determining the heat generated by a typical combination lamp and luminance. (XBB 855-4074)

Progress in FY 1987 included gathering basic information on luminance types and lighting distributions, types of control systems and the variables needed for utilization of visual performance and visual comfort metrics. Workspaces were examined to locate a one with a good balance of reality, complexity, and feasibility for the Lumen-Micro program.

Computer Imaging

Computer logic has been developed capable of presenting visual images of illuminated spaces. The images show how different lighting equipment and techniques can change the appearance of illuminated spaces. The program has been developed to handle specular and diffuse reflecting surfaces. It can also handle complex objects in the space. An initial validation for simple spaces was performed by comparing luminance results with Lumen-Micro, a commercially available program that also computes luminances, but only for empty rooms with purely diffuse reflecting walls. Further validation is required based upon physical measurements of real interior objects such as furniture. (see Fig. 3).

Thermally Efficient Luminaires

Several years ago we demonstrated that luminaire performance could be improved by applying multiple dielectric coatings to reflecting surfaces. Further work was directed toward understanding the thermal performance of luminaires. It was found that fluorescent lamps in most fixtures operate well above the optimum temperature, which decreases light output and system efficacy. In a pilot study during FY 1987, we have shown that air handling luminaires can increase light output by as much as 20 percent. Demonstrations have shown that proper venting of enclosed ceiling mounted fixtures can increase output and efficiency by 15 percent.

Peltier Device

Virtually all fluorescent lamps in fixtures operate at temperatures above the optimum, which decreases light output and efficacy by 15 to 20 percent. A Peltier Device has been used to control lamp wall temperatures and reduce losses. The current systems are designed to be positioned on the external surface of the lamp wall. This design has been as a useful tool in the laboratory for characterizing fluorescent lamp systems.

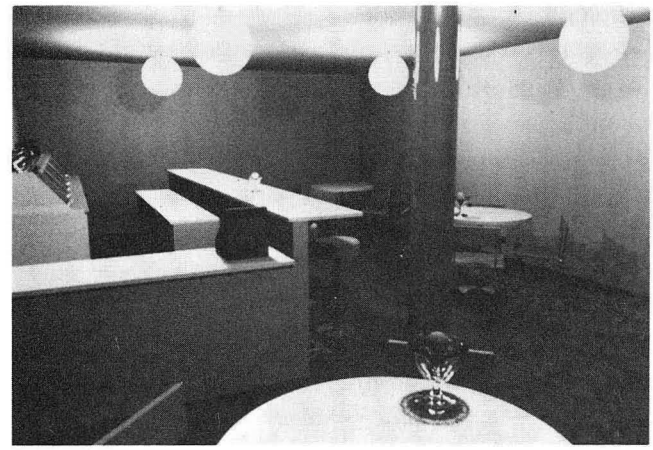

Figure 3. A computer generated "photograph" of an ice cream parlor. (CBB 878-6585)

Planned Activities for FY 1988

Advanced Lighting Design

During FY 1988 these elements will be brought together and a complete assessment of the totality of lighting factor will be performed. Cost of lighting energy, as well as costs of providing a given level of performance and comfort will be established, as will their sensitivity to choices of technical lighting system parameters.

Computer Imaging

The principal activity for FY 1988 will be the validation of the imaging logic for complex objects. In cases where directional reflection coefficients for surfaces are known, a direct comparison can be readily made. However, we expect that known coefficients are not sufficiently representative and part of the FY 1988 effort will be devoted to measuring these coefficients for selected typical indoor and outdoor surfaces. This effort will need some equipment development.

Thermally Efficient Luminaires

The principal effort will be devoted to determining methods for introducing convective cooling in four-lamp, wrap-around, ceiling-mounted fixtures. We will determine the quantitative benefits of various technical and strategies. Considerable effort will also be expended to upgrade and rehabilitate the thermal test chamber, which has deteriorated during

the past year. Calibration, painting, and improved photocell systems will be part of this rehabilitation.

Peltier Device

In a potentially more practical system the device would be an integral part of the lamp, and could be driven by the ballast. Further research will develop such a Peltier Device. A number of technical problems will be examined in FY 1988. In particular, the size and geometry of the Peltier Device system needed to cool and maintain a 40° C temperature in a four-foot fluorescent lamp will be determined along with specification of the required electrical power, voltage, and current range of operation.

Subsequently, we will begin constructing of an experimental test set up in which the environment of a Peltier Device in a lamp can be simulated. This test set up will facilitate measuring of the required performance of the Peltier Device, and determine the amount of heat to be dissipated, and the means to drive the device. Possible methods of dissipating the heat from the Peltier Device located in the lamp will be examined, based on the electrical requirements for operating the Peltier Devices. A system will be designed that provides the Peltier Device power and is compatible with a core or an electronic ballast.

IMPACTS OF NEW LIGHTING TECHNIQUES ON PRODUCTIVITY AND HEALTH

The idea that lighting might negatively affect health has appeared often in the lay press during the past few years. Scientific data are lacking, especially to ascertain whether new energy-efficient technologies adversely affect human health and productivity.

Performance and productivity may be influenced by the lamp electronics and associated controls, the fixture, or the geometry and location of the lighting system. We classify these lighting factors as: color variations; glare; intensity fluctuations; spectrum variations, including the ultraviolet region; electromagnetic fields generated by the lamp, ballast, or controls; and flicker. All of these could evoke a variety of human responses (behavioral, psychophysical, physiological, or biochemical).

Our research seeks to assure that new energy-efficient lighting technologies do not adversely affect human health and productivity. We are investigating whether any aspect of new technologies can produce responses in humans. If we identify responses, we will characterize the effects and identify the necessary changes in lighting technologies. Although subjective responses of workers provide some information, such responses are generally confounded by a mix of sociological factors and individual motivations. The investigations carried out by LBL use objective responses to establish cause and effect, and ensure repeatability.

The impacts program is divided into two areas: (1) direct effects of lighting on the human autonomic system (carried out at University of California, San Francisco and LBL), and (2) interactions of lighting that affect visual performance and productivity or comfort (carried out at the UC School of Optometry and LBL), which are termed here "lighting ergonomics".

In the first area of this program, lamps to be evaluated include: incandescent, cool-white fluorescent, high-pressure sodium, and metal halide. Human responses to various lighting conditions will be assessed by monitoring autonomic responses, including heart rate, galvanic skin response, muscle strength, exercise tolerance, facial expression, and pupillary response. Behavior measures to be used include memory (Wechsler Memory Scale and Sternberg's Memory Scanning Time), cognitive function (mental arithmetic), time estimation, and simple reaction time. Other behavioral tasks will probably be included.

Data-gathering and subject control are supervised by trained medical personnel. A national technical advisory committee oversees and reviews the project. First results of this effort concern the effects of visible-spectrum and low-frequency radiation on human muscle strength, and, as described previously, they indicate that psychological factors are the likely cause of reported effects. A second set of experiments using pupillometry has, however, shown very robust and surprising effects of spectrum on pupil responses to different lamps.

The second area of this program studies primarily issues of glare resulting from lighting systems, and, to a lesser extent, flicker. In addition to these principle concerns, theoretical studies and comparative analysis are undertaken on models of visual performance particularly as they relate to understanding the benefits of more energy-efficient lighting.

Present knowledge and prescriptions by the lighting community for dealing with glare are based on subjective responses, without support by objective criteria. It is reasonable to implicate pupil responses as relevant to glare discomfort since pain receptors are present in the iris and the nervous pathway necessary to signal pain is present in the fifth trigeminal cranial nerve. Some studies by vision scientists have suggested pupil response as a possible to the sensation of discomfort but this conclusion is not

generally accepted in the vision community. We have undertaken a series of studies to clarify the possibility that pupil dynamics can be used as an indicator of glare response.

Accomplishments During FY 1987

Direct Effects of Lighting on the Human Autonomic System

Accomplishments for FY 1987 were in methodological studies, brightness studies, and PC computer development. The methodological studies primarily addressed validation of our pupillometer, including the effects on the pupilometer's accuracy resulting from test lamps; determining reliable threshold settings of the pupilometer in order to understand and avoid possible erroneous measurements because of conflicting or antagonistic threshold settings; exploring potential effects of eye movement on area measurement; examination of behavioral effects such as the subject initiating data collection by pressing a button; and potential effects of subject viewing a color verses black and white television. Several pilot studies led to two subjective brightness studies, both designed to correlate pupil size to subject report of brightness between metamerically matched pairs of fluorescent lamps over a range of low intensities; a second study looked at a range of higher intensities.

Summary of Methodological Studies

1) *IR Studies.* Several pilot studies designed to evaluate effects of additional infrared energy on the output of the MMI pupilometer were accomplished. These studies evaluated various combinations of lamps, especially those with high IR content such as High Pressure Sodium with and without an additional IR source lamp for the MMI on various threshold settings of the instrument. The results indicated the lamps used, and those expected to be used in this research, all failed to introduce sufficient IR energy to effect the output of the MMI under normal operation.
2) *Threshold Effects on the Pupilometer.* Studies were designed to explore the range of various threshold and sensitivity settings of the MMI in order to establish optimum settings, and define the outside limits of these settings to ensure accurate operation of the instrument.
3) *Eye Movement Studies.* Studies were implemented to determine whether eye movement affected the area recording of the instrument, and, if so, what range of eye movement is tolerable. The results indicate that eye movement of less than ten degrees vertically and horizontally failed to alter the area output. Movement greater than 15 degrees produced artificial changes in the area output.
4) *Behavioral or Button Press Studies.* Two variables in our methodology were suspected of contaminating the dependent variable (average pupil size over time); instructions to the subject to press the button (initiating the data collection period), and the performance of pressing the button. Results of these studies showed a systematic pupillary dilation just prior to pressing the button (anticipatory response), with the approximate amplitude of 0.4 mm diameter and a return to baseline in approximately 2.5 seconds. This response appeared to habituate over repetitions.
5) *Color Versus Black and White TV Viewing.* We anticipate evaluating visual performance under various lighting conditions with a contrast sensitivity task utilizing a black and white monitor. Therefore, we wanted to compare its effects to those of a previously used color monitor. The results indicate the black and white monitor used in this study emitted intermittently high levels of scotopic intensity. This emittance of large scotopic intensity is in direct conflict with our research concerning the scotopic/photopic ratio of various lamps.

Summary of Subjective Studies

1) *Low Range Intensity Study.* This study investigated the correlation between pupil size and subjective report of brightness, comparing photopically matched pairs of metamerically matched lamps across three intensities. The results showed a strong relationship between subjective report of brightness and pupil size elicited by scotopic intensity, and compared to photopic intensity.
2) *High Range Intensity Study.* This study was similar to the above study except the intensities chosen were individualized from a calibration procedure, to establish each subjects' scotopic response curve, and referenced to a higher intensity level. The results were consistent with those above in that there was a high correlation between pupil size and subjective report of brightness.

Summary of Computer Development

A Sperry PC computer was installed. Some of the necessary hardware includes Scientific Solutions

LabMaster Board, 16 A/D, 16 D/A, 24 I/O Scientific Solutions DADIO Board, and 24 I/O. Software installed includes: ASYST, Scientific Solutions LAB-PAC, GW BASIC, Turbo PASCAL, and Microsoft C. In-house software developments include: data acquisition, storage, retrieval, reduction, transfer, and blink and block removal programs.

Lighting Ergonomics

Visibility Studies. Cost benefit studies can be a basis for establishing recommended illumination levels. We have studied the present Illuminating Engineering Society recommended levels and written a detailed report. The results suggest that recommended illumination levels for the young population are too high, and that they underestimate the important parameters to be considered, such as the cost of light and the value of visual work.

A comprehensive review of lighting research with respect to lighting quality was completed, and a draft research agenda was prepared and is being critiqued. Components for the luminance mapper have been selected and assembly of the system will begin next fiscal year.

In addition, an educational article appearing in the Journal of Lighting Design and Application titled "To Average or Not To Average" was published.

Glare Studies. The pupil undergoes small, uncontrolled oscillations known as hippus, or generally, pupillary unrest. These oscillations and their associated frequency spectrum could be affected by the presence of glare, especially as the different pupillary pathway is affected by the kind of ocular discomfort associated with glare. In order to examine this issue, studies have been initiated to clarify the nature of pupillary unrest, since existing information is contradictory.

Flicker Studies. A prominent difference between hard copy and the visual display terminal is that the letters on the VDT screen are constantly being refreshed electronically at a rate of 60 Hz. Thus, a VDT viewer is exposed to a flickering light signal that is generally not perceived as flickering because the repetition rate is beyond the critical fusion frequency (CFF). (Exceptions could occur under conditions of reverse video and very high contrast.) Evidence using cortically evoked potentials on higher vertebrates indicates, however, that frequencies even higher than 60 Hz are being processed in the visual pathway. We are presently using the techniques of electroretinography to investigate whether the human retina is responding to the flickering VDT screen synchronous to the refresh rate. Because the signal strengths to be measured are of a quite small fractions of microvolts, we refresh the VDT at frequencies slightly above and below 60 Hz in order to reduce the effect of the ubiquitous 60 Hz environmental background in buildings. Further attention to this problem is necessary as the VDT electrons, upon striking the phosphor, produce a radiating magnetic field that escapes even additional VDT shielding. Preliminary results using extensive data averaging techniques on information from one subject indicate a weak but definite response.

Planned Activities for FY 1988

Direct Effects of Lighting on the Human Autonomic System

Three principal efforts will be undertaken during FY 1988. First, a more detailed study of the factors that influence the variance in the pupillary measurements so we can establish the number of subjects necessary, and the length of times of a subject run for a particular accuracy. Incorporated into this effort is a new study of the effect of spectrum on pupil size, which uses metameric sources, i.e., sources with equal color but designed with different ratios of scotopic to photopic luminance. This study would eliminate any concerns about to color differences that were present as a possible confounding condition in the previous experiment, where incandescent and high-pressure sodium lamps were compared (see Fig. 4).

The second effort will be a comparative examination of effects on visual performance under conditions of equal photopic luminance, but different scotopic luminance, and, therefore, different pupil sizes. Visual performance will be studied by the use of grating contrast sensitivity determination using the computerized spatial frequency testing system previously developed.

The third activity in this area is the completion of the construction of the pupil stimulator to be used in conjunction with the pupilometer system. This instrument is designed to provide the viewer with a slowly varying scotopic luminance under conditions where the photopic luminance is kept constant. The previous pilot studies have shown that scotopically richer sources appear subjectively brighter. Using pupil stimulator we can determine both whether the perception of brightness is correlated with pupil size, and, by studying time-varying scotopic luminances, to what extent perception of brightness is in phase with pupil.

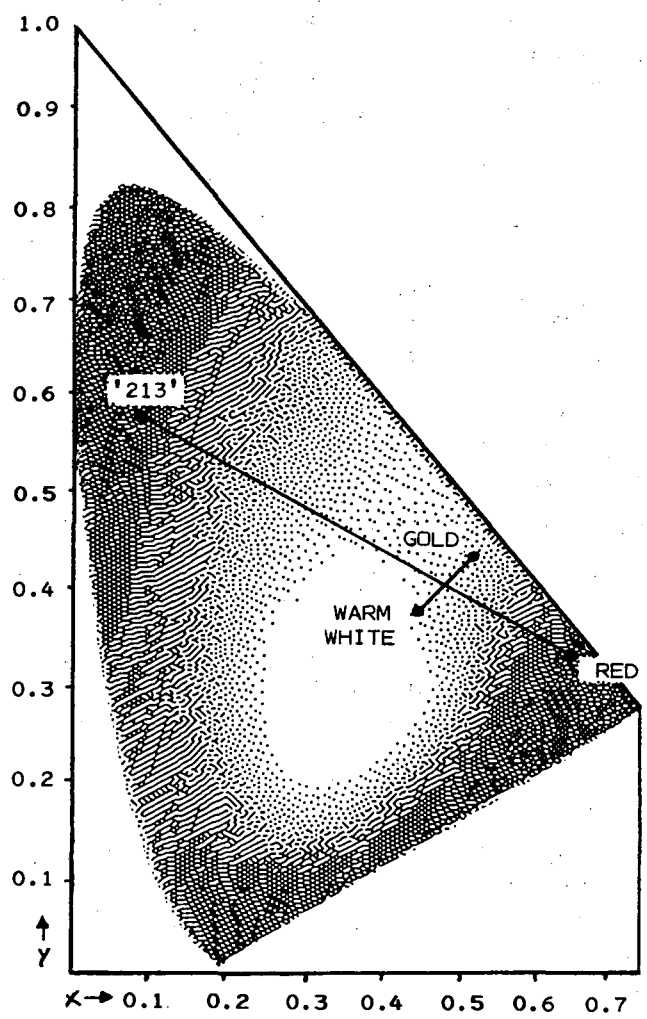

Figure 4. Chromaticity diagram displaying scotopically rich and deficient metameric combinations. (XBL 8712-5381)

Lighting Ergonomics

Visibility Studies. A number of on going efforts in this area are designed to obtain a verifiable, quantitative, and comprehensive methodology for prescribing illumination levels in the workspace. During FY 1988 the focus will be on three principal areas: completing the cost benefit report for publication, constructing an operating luminance mapper, and completing the size methodology analysis as an indicator of visual performance potential. The report on using cost benefit analysis to study the consistency of the lighting recommendations of the Illuminating Engineering Society will be prepared for journal publication. Computer, photographic, and photometric hardware will be assembled as the first configuration of the luminance mapper, and a calibration study will be undertaken. The statistical analysis leading to the universal scaling law resulting from the Bailey data (which uses the ratio of target size to acuity limit as a the metric for visual performance potential) will be completed. This universal scaling is expected to have a radical effect on field procedures for establishing adequacy of workspace illumination. This effort, coupled with the field measurement capability of the luminance mapper, will provide for the first time a very major step in the ability of lighting users to effectively quantify their luminous environments.

Glare Studies. The analysis of the shape of the pupillary unrest (hippus) frequency spectrum will continue. The spectrum under conditions of discomfort glare will be compared to the spectrum in the absence of discomfort glare. The results of the work on the discovery of beat effects on pupillary response, along with a model analysis, will be written for journal publication. The modeling effort makes use of the non-linear logarithmic response of the mean pupil size to changes in light level to compactly describe the connection between the frequency dependent reduction in mean pupil size and the amplitude of the beat response.

Flicker Studies. Work will continue on the electroretinogram response to VDT flicker and several additional subjects will be tested. Should the responses of those additional subjects mimic the results of the previous subject, the combined results will serve to establish a new effect, and these efforts will be written for journal publication.

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INDOOR ENVIRONMENT PROGRAM

INTRODUCTION

LBL is a major center of building science research. An important part of that research is the environment defined by the building -- the major focus of the work of the Indoor Environment Program. The Program examines the scientific issues associated with the design and operation of buildings to optimize building energy performance and occupant comfort and health.

Optimizing health and comfort of occupants is addressed in different ways by the groups that comprise the Program. The Energy Performance of Buildings Group examines energy flow through all elements of the building shell. It measures air infiltration rates, studies thermal characteristics of structural elements, and develops models of the behavior of complete buildings. The potential for savings in the infiltration area is great. The heat load associated with natural infiltration is about 2.5 quads/yr costing about $15 billion annually. It may be economic to reduce this by 25%.

This change, however, may produce undesirable effects in the environment of the building. Since ventilation is the dominant removal mechanism for pollutants found within buildings, concern continues about the impact of designs or changes in operation that lead to its reduction.

This issue has been an important theme for the work of the other projects of the Program. Efforts include characterizing the emission of various pollutant classes from their respective sources, studying the effectiveness of ventilation in removing pollutants from indoor atmospheres, and examining the nature and importance of chemical and physical reactions that can affect the occurrence and amount of airborne pollutants. The Program has projects that have concentrated specifically on three major pollutant classes: combustion products, arising from indoor heaters and other combustion appliances; radon and its progeny, arising from materials that contain radium, a naturally occurring radionuclide; and formaldehyde and other organics, arising from a variety of building materials and furnishings. In addition, the Ventilation and Indoor Air Quality Control and Energy Performance of Buildings projects investigate techniques for controlling airborne concentrations, develop devices for monitoring pollutants in laboratories and buildings, and design or carry out field surveys of energy use and indoor air quality in residential and commercial buildings. The Indoor Exposure Assessment project also devotes time to assessing the health effects of indoor pollutant exposures.

It is difficult to generalize the results of on-going research efforts. However, there are several important hypotheses that have evolved from this work that we continue to explore as this research proceeds.

A. **Air quality in buildings is dominated by sources.** Problems that have been seen are more often related to strong indoor sources than to deficiencies in ventilation.

B. **Air pollution is a buildings problem.** The concentrations of pollutants observed within buildings are comparable to those outdoors (when major indoor sources are present, the concentrations indoors are substantially higher). Since people spend 70-90% of their time inside buildings the major portion of their exposure to air pollutants occurs within buildings. Therefore, because sources and removal processes are often associated with building structure and operation, we work from a perspective that air pollution is a buildings problem.

C. **Ventilation is the best control strategy for indoor pollution within a building.** Ventilation using outdoor air affects all indoor pollutants in a similar way. Therefore, it is the best single strategy to employ in buildings for pollutant control. This assertion does not contradict statement A above. Rather, it acknowledges that we do not know and cannot identify all the pollutant sources in a building. If a particular pollutant is known to be a problem, the source of the pollutant should be treated. Since such information is usually lacking, ventilation remains the best general indoor pollution control strategy.

Indoor Radon*

R.G. Sextro, A.V. Nero, K. Garbesi, J. Harrison, J. Hill, D.D. Lee, C. Loureiro, B.A. Moed, W.W. Nazaroff, T. Nuzum, R. Prill, K.L. Revzan, and B.H. Turk

Key elements of the research conducted by the Indoor Radon group are to 1) provide a method of predicting or identifying geographical areas where houses with elevated indoor concentrations might be found; 2) to improve understanding of the mechanisms for production and transport of radon through soils and into buildings; 3) to identify, develop and investigate means of controlling high indoor radon concentrations; and 4) to study the behavior of radon progeny under a variety of indoor environmental conditions.

ACCOMPLISHMENTS DURING FY 1987

Soil as a Source of Indoor Radon

Because soil appears to be the principal source of radon in the indoor environment, particularly in those homes with elevated concentrations, studies of soil and soil properties have been integrated into several projects. One aspect of this research is the use of national data on surficial radium concentrations from the National Airborne Radiometric Reconnaissance This data set and our preliminary work with it are described in more detail in an earlier Annual Report.[1] Current efforts are focussed on assessing the degree of variability in the radium concentration in the surface soil within specific regional or geographic areas, and for the country as a whole. In this latter regard, a preliminary national map has been constructed from the data set, as shown in Figure 1. The data initially gridded at ~1.6 km intervals along the flightlines are regridded to larger, 20 × 20 km spacings in order to provide a map at a usable scale. It is apparent from this map that there are significant regional variations in the radium content of surface soils. In some cases, occurrences of houses with elevated indoor radon concentrations can be broadly associated with these areas. Examples of such areas are eastern Pennsylvania/northern New Jersey and eastern Tennessee/western North Carolina. In other situations, the association between apparent radium content and indoor radon is unknown or not as straightforward. One such example appears to be the relatively high mean indoor radon concentrations in the Fargo, ND area, yet the map suggests that the soil radium concentrations are not elevated significantly.

It is also apparent from the map that calibration anomalies exist between different areas, partly due to the fact that seven different subcontractors were used to collect the aerial radiometric data. Further, there are areas for which the data set contains no data, as indicated by white areas on the map, although most of the quadrangles covering the conterminous U.S. were flown. These problems will be investigated further. Smaller-scale maps for 1° × 2° quadrangles have been produced for selected areas, and offer the possibility of more detailed investigation of the relation between indoor radon and soil radium. Descriptive statistics for each quadrangle area have been compiled and again indicate considerable variation in the radium distribution by region.

Measurements of soil properties around homes have been conducted in conjunction with two field studies of indoor radon. Of particular interest has been both soil radium concentration and air permeability, conducted *in situ*. In the case of studies conducted in the Spokane, WA area, soil air permeabilities were of the order of 10^{-11} m^2, with about a factor of 5 range in these values. The emanating radium content of the soil ranged from 4.4 to 8.8 Bq kg m^{-1}, and the mean soil gas radon concentrations showed a similarly narrow range over 23 sites, from 10.9 to 24.9 kBq m^{-3}.[2]

In contrast to these measurements, soils in the vicinity of the seven study homes in New Jersey exhibit considerably greater variation in air permeability and soil gas radon concentration, both from site-to-site and within a specific site. Based on preliminary data from one home site, the soil permeabilities ranged over 4 orders of magnitude, from 1 x 10^{-8} to $< 10^{-12}$ m^2. Soil gas radon concentratons varied from ~13 to over 3300 kBq m^{-3}, a range of more than 2 orders of magnitude. While this heterogeneity is not surprising, it does indicate that efforts to characterize radon-related soil parameters, either locally or regionally, must be done with caution.

*This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Office of Building and Community Systems, Building Systems Division, and by the Director, Office of Energy Research, Office of Health and Environmental Research, Human Health and Assessments Division and Pollutant Characterization and Safety Research Division of the U.S. Department of Energy under contract No. DE-AC03-76SF00098. It was also partially supported by the Office of Environmental Engineering Technology Demonstration, Office of Research and Development, U.S. Environmental Protection Agency through Interagency Agreement DW89931876-01-0 with DOE, and by the Office of Radiation Programs, Office of Air and Radiation, U.S. EPA through Interagency Agreement DW89932609-01-0 with DOE.

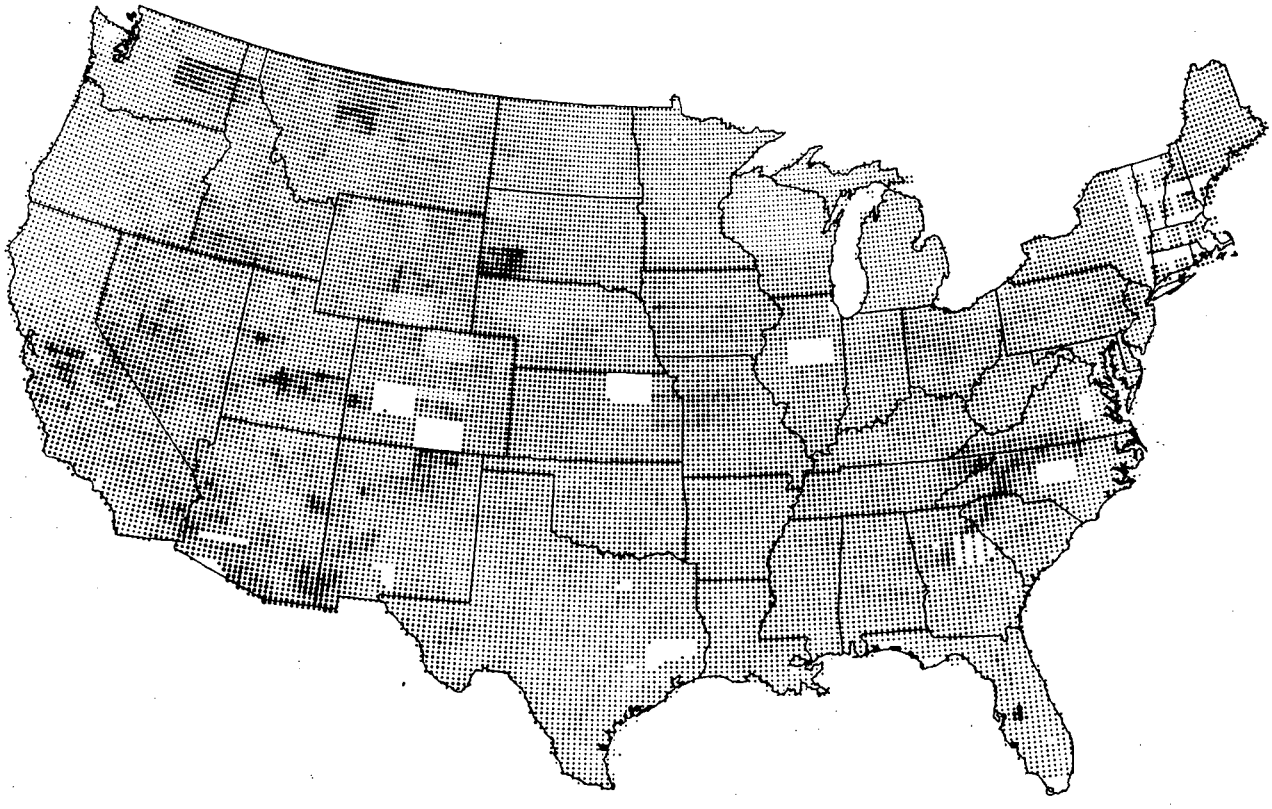

Figure 1. Mean surficial soil radium concentrations for 20 × 20 km areas of the coterminous U.S. compiled from NURE data. The dots vary in size, representing 6 radium concentration intervals: 0 - 20, 20 - 40, 40 - 60, 60 - 80, 80 - 100, and > 100 Bq kg^{-1} of soil [XBL-8711-4927A]

One area of new research recently undertaken by both the Indoor Radon and Indoor Organics groups is the application of research on soils and soil gas transport to studies of the movement of volatile organic compounds through soils and into buildings. There is evidence that in some homes located near municipal land-fill dump sites, soil gas transport may be a source of indoor VOCs. Results of our initial research are described in the chapter on Indoor Organics in this annual report.

Intensive Seven Home Study of Radon Entry and Control

Work was begun during FY86 on a detailed study of radon entry and removal in seven homes in New Jersey.[3,4] There are four components to this research: 1) house and site characterization measurements, 2) continuous monitoring of radon and environmental parameters, 3) diagnostic procedure development, and 4) installation and operation of selected radon reduction techniques. Field work was completed in the homes at the end of FY87 and final reduction and analysis of the data begun. The seven homes chosen for the study were located in north-central New Jersey, within a 25 km radius of Chester, NJ. These houses were one- or two-story detached frame houses with basements. The basement walls in each case were constructed of hollow-core concrete or cinder block. Forced-air heating systems were used in all but one house, where a hot-water heating system was employed. Initial (pre-mitigation) indoor radon concentrations ranged from 700 to 7600 Bq m^{-3} in the basements and from 480 to 2500 Bq m^{-3} in the living space of the homes.

A sampling of data from house LBL11 is illustrated in Figure 2. These data were acquired during a two-week period in November 1986, before mitigation systems were installed in the home. As can be seen, the first three curves—basement radon concentration, pressure difference across the basement walls, and indoor-outdoor temperature difference—appear to behave in a similar manner. The basement radon concentration varies by more than a factor of five within a 2 day period, and exhibits a diurnal variation extending for most of the two week

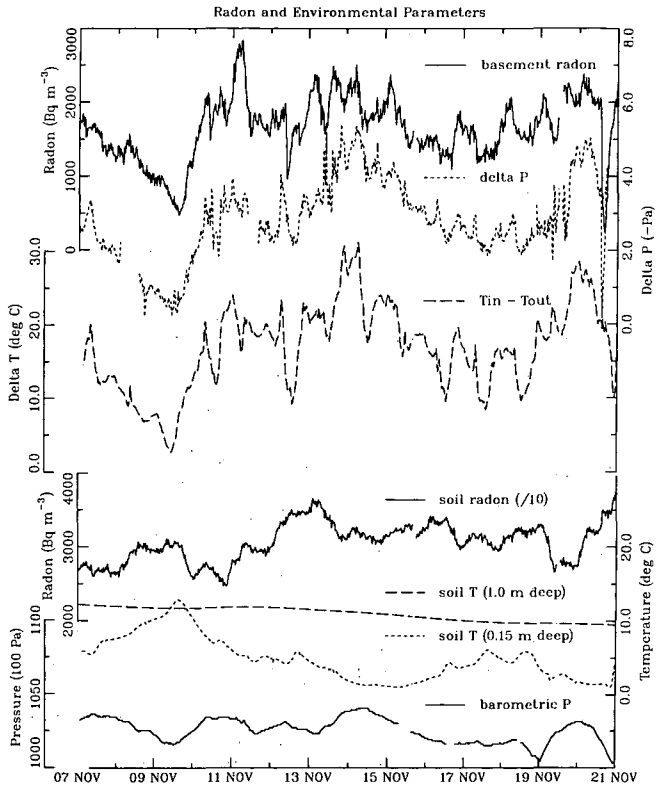

Figure 2. Continuous data on radon concentrations and environmental parameters during a two-week period in November 1986. The data interval is every 30 min. Note that in the case of the differential pressure data, the axis label is in terms of negative pressure. |XBL-873-1256|

period. These same patterns have been observed in some, but not all, of the houses in this study for much of the measurement period.

The average differential pressure between the basement and outside the building shell at ground level has been plotted so that an increasing negative pressure difference is shown as an upward change in the curve. These data exhibit variations similar to the radon concentration data, as does the difference between the indoor temperature at the first floor and the outside temperature. The indoor-outdoor temperature difference is one of the driving forces (the thermal stack effect) responsible for the pressure difference across the building shell. Wind loading on the building shell also contributes to the pressure difference, and might help explain some of the detailed differences in these curves. These data appear to confirm, at a general level, the importance of convective soil gas flow into buildings as a source of indoor radon.

Data from four of the other houses appear to follow a similar pattern, showing a correspondence between the temperature and pressure differentials and the resulting basement radon concentrations. In two of the houses, the preliminary data analysis indicates that peaks in the basement radon concentration apparently lag the corresponding increase in differential pressure, in some cases by a few hours.

Also shown in Figure 2 are radon concentrations in the soil gas, monitored continuously via a probe inserted through the basement floor, soil temperatures measured at two soil depths at a location approximately 1 m from the house, and the barometric pressure data for the same period. Neither the barometric pressure nor the soil-gas radon levels appear to be associated with observed fluctuations in basement radon concentrations. As can be seen, the soil temperatures show a slight downward trend during this two week period, which was a time of seasonal change in the weather.

Another aspect of this research has been the development and evaluation of a series of diagnostic procedures for identifying the specific means by which radon enters a given house, in order that suitable remedial radon reduction measures can be prescribed and installed.[5]

A general approach for radon diagnostics is shown in Figure 3. The premise for much of this

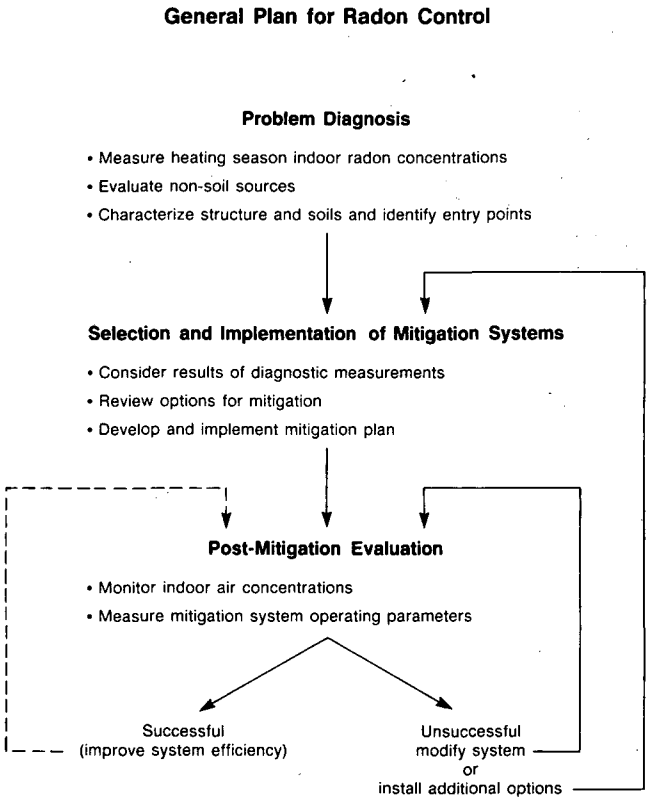

Figure 3. Schematic of a general approach to radon diagnostics and control. |XBL-871-8920|

discussion is that pressure-driven flow of radon-bearing soil gas is the most significant source of radon in houses with elevated radon concentrations, although the procedures do include a general evaluation of non-soil sources, such as water or building materials. An important step in the process is to determine or verify that the average indoor radon concentrations are above guideline values. Because indoor radon concentrations vary with as illustrated in the previous discussion, short-term measurements (< 4 days) are often not adequate to eliminate the possibility of false positives or negatives. This topic is also discussed below in another section of this report. Aspects of control strategies are also discussed in.[6]

Initial evaluation of a house with elevated indoor radon concentrations is based on visual inspection to help locate potential soil gas entry locations. The inspection process is augmented with a building survey questionaire, which can provide further detail and information on potential entry locations, leading ultimately to the specification of a suitable radon control system. In addition to the survey and inspection, tests of air flow communication below the basement floor slab are performed by drilling small holes through the slab at several locations and using a heavy-duty industrial or shop-type vacuum cleaner to depressurize the area below the slab. In this way, the permeability of the subslab zone can be measured, which is important information in assessing potential radon entry locations as well as in determining the viability of using subslab ventilation as a radon mitigation technique.

Alpha-scintillation (Lucas) cells are also important diagnostic tools in evaluating possible entry areas. Samples can be obtained from specific building zones, or using a small volume probe, from behind or within walls, drains or other areas that would indicate possible entry locations. In some cases, the use of a blower door to depressurize the building to ca. -10 Pa will assist in locating entry points. At greater depressurization, air flow through small cracks or other suspected entry points can be visualized with the aid of chemical smoke from commercially available smoke tubes. In some situations a hot wire anemometer may be used to quantify the amount of air movement into the building shell.

A blower door is also useful in determining the effective leakage area of different parts of the building structure. This information is important in establishing the leakage across the building substructure, where soil gas entry is likely, and the leakage of the building superstructure, which helps determine the natural ventilation rate of the building. This latter element can be important in the selection and sizing of heat recovery ventilation or basement pressurization as radon reduction methods.

Certain types of appliances or heating systems can add to the depressurization of the building substructure. By using a sensitive differential pressure instrument, the effect of the operation of these appliances or furnaces may be determined. Forced-air furnaces are very often a source of additional substructure depressurization, largely through leaky return air ductwork or the furnace cabinet itself. The thermal column established by the combustion exhaust through the furnace chimney may also add to the negative pressures. While these are important winter-time sources, attic or whole-house fans may also depressurize the house at times when the furnace system is not used.

Modeling Soil Gas Transport

Because pressure-driven flow is largely responsible for radon entry into buildings, especially those with elevated indoor radon levels, a theoretical model has been developed to simulate this phenomenon.[7] Based on a three-dimensional, finite difference computer code, the model incorporates 1) the generation and decay of radon within the soil, 2) radon migration through the soil due to diffusion and convective flow induced by the pressure difference developed across the building shell, 3) entrance of soil gas into the building via an assumed peripheral crack system at the basement floor-wall joint, and 4) the resultant indoor radon concentration.

Mathematically, the model first establishes a pressure field in the soil surrounding a house with a pressure differential, ΔP, across the building shell. A detailed discussion of the mathematics and the derivations are provided in another report;[7] the main elements of the approach are only summarized here. Using Darcy's law and the continuity equation for the mass balance for the soil gas, one obtains a general expression for the induced pressure field in the soil:

$$\vec{\nabla}\cdot(k\vec{\nabla}p) = 0, \qquad (1)$$

where k is the air permeability at point (x,y,z) in the soil and p the induced pressure at the same point. The soil gas velocity field in the soil is then given directly by Darcy's law, namely:

$$\vec{q} = -\left(\frac{k}{\mu}\right)\vec{\nabla}p, \qquad (2)$$

where μ is the dynamic viscosity of soil gas. Finally, the flux of radon through the soil is then given by the sum of convective and diffusive flow, where the diffusion term includes both a molecular diffusion term and a mechanical or hydrodynamic dispersion term. Specification of radon migration through the soil under steady-state conditions then allows one to evaluate both the steady-state radon concentration field in the soil, and the resulting radon entry rate into the building.

Numerical methods are used to solve the second order, linear partial differential equations for both the pressure and radon concentration fields, using a finite difference technique employing a discretization method. In order to simplify the task, three zones of permeability are established in the soil block surrounding the house. Within each zone, the permeability is assumed to be constant. These zones correspond to the bulk soil block, a region or layer adjacent to the walls, and a separate region beneath the floor slab. The thickness of these layers adjacent to the building shell can be specified. These separate regions are consistent with actual construction techniques. Next to a basement wall is a region that is backfilled with soil after the wall has been built which often has a higher permeability than the surrounding 'undisturbed' soil. In many houses, an aggregate layer is also established below the basement floor before it is poured in place.

The model allows specification of a number of parameters, including the spatial dimensions of these various permeability zones, the pressure difference across the building shell, and the physical dimensions of the crack system through which radon enters the building. By varying these parameters, the sensitivities and importance of these effects have been investigated. As one example, since the total entry rate of radon into the structure is a combination of the diffusive and convective fluxes, the importance of each component has been evaluated for different soil permeabilities and applied pressures. The results suggest, as expected, that the diffusional component has greater importance for low permeabilities and low applied pressures and that this diminishes with increasing permeability and/or applied pressure. At higher flows, the diffusion component is actually reduced, because the radon concentration gradient at the crack-soil interface is reduced.

Examining the effects of crack width and soil permeability on the pressure field indicates that crack size is important for low permeability soils, but for higher permeabilities, only the smallest crack dimensions affect the pressure field. An example of the calculated pressure profile in the soil is shown in Figure 4 for a crack width of 0.5 mm and a high soil permeability (10^{-10} m^2). A comparison of this result with that for a much lower soil permeability (ca. 10^{-14} m^2) shows that the pressure gradient in the soil is contracted toward the crack as permeability increases. This is due to the fact that flows increase as permeability increases, and the pressure drop across the 0.5 mm gap increases as well, thus reducing the pressure drop in the soil itself. At crack widths greater than 5 mm, the variation in soil permeability has little effect on the pressure gradient in the soil.

Similar analyses can be done for steady-state radon concentrations in the soil. One example is shown in Figure 5 for a very high permeability soil.

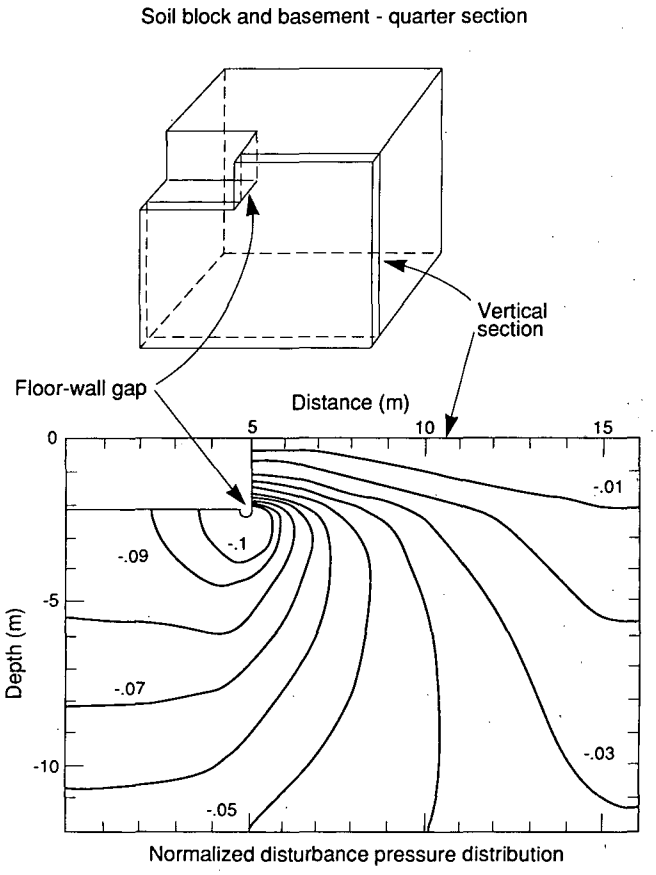

Figure 4. Modeling results for soil pressure gradient. The top portion of the figure is a schematic representation of the basement and the soil block in which it sits. The location of the vertical cross section presented in the lower portion of the figure is indicated. Due to symmetry, only a quarter of the basement and soil block is modeled. The lower portion of the figure shows profiles of the pressure field in the soil surrounding the basement. A 0.5 mm gap between the wall and the floor is assumed, and the soil permeability is 10^{-10} m^2. [XBL-886-11002]

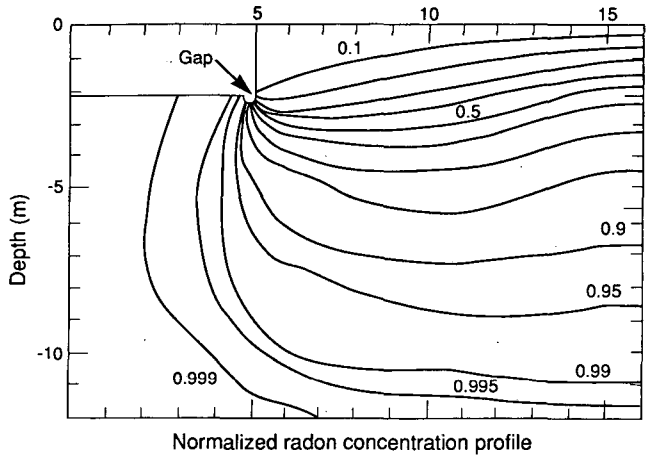

Figure 5. Soil gas radon concentration profiles for the same vertical cross section as indicated in Figure 6. The gap width is 5.0 mm and the soil permeability is 10^{-9} m^2. |XBL-886-11003|

As the figure indicates, the presence of the house affects the soil gas radon concentration at a distance of several meters away from the basement wall. As soil permeability decreases, the effect is less pronounced.

The model has allowed investigation in a systematic way of the interactions among various soil and house parameters. These analysis will be useful in interpreting experimental data obtained in actual houses, and in turn, some of the experimental data can be used to provide validation of components of the model.

The Response of Charcoal Detectors to Varying Radon Concentrations

Radon adsorption by charcoal is the basis for passive sampling devices that provide both an easy and inexpensive method of obtaining quick diagnostic measurements of ^{222}Rn levels. This method is well suited to γ-ray counting and typically requires exposure times of only a few days, unlike α-track devices with recommended exposure times of at least a month. But because Rn desorbs from charcoal as well as it adsorbs onto it, the response of charcoal-based passive samplers to time-variant Rn levels is an important consideration, especially in light of the evidence that typical Rn concentrations undergo diurnal as well as seasonal variations, as illustrated in Figure 3 above.

Two main types of charcoal-based passive samplers have been introduced, an open-faced device and one that incorporates a diffusion barrier that limits the rate of radon accumulation by the device, and at the same time, restricts the back diffusion rate of radon from the device. The operation of these devices, particularly under conditions of varying radon concentration, is not well characterized. Stimulated by our observations of diurnally-varying radon concentrations in homes we have undertaken a study of the the integrating characteristics of charcoal-based radon detectors.[8]

Models describing radon adsorption and desorption by charcoal canisters, both open-face and diffusion-limited, have been assembled. A detailed discussion of the modeling is provided in another report.[8] In general, the models are based on solving the one-dimensional diffusion equation,[9]

$$\frac{\partial y}{\partial t} = D\frac{\partial^2 y}{\partial x^2} - \lambda y, \quad y = f(x,t). \tag{3}$$

where x is the height in the charcoal bed above the bottom of the canister, y(x,t) is the concentration of ^{222}Rn in the charcoal, t is the time, D is the diffusion constant, and λ is the radioactive decay constant for ^{222}Rn.

Assuming that the lid is taken off at time zero, and that the canister previously had no ^{222}Rn in it beforehand, the initial condition is then $y = 0$ for all x. Additional boundary conditions at the bottom of the canister and when the top is exposed to the Rn in the environment are imposed to help solve the series of equations.

Employing a technique of using a series of linear functions to describe the time-varying radon concentrations in air along with separation of variables, one arrives at a series solution to y(x,t). Hence, knowing y(x,t) for all t, the total amount of ^{222}Rn in the canister at any time T_0 can be found by integrating across the thickness of the charcoal bed.

In the case of the diffusion-limited devices, the picture of the diffusion barrier was simplified somewhat in order to utilize the one-dimensional solution derived for the open-face device, described above. By assuming air in the immediate space after the diffusion barrier and just above the charcoal bed is well mixed and that the diffusion barrier connecting this space with the outside air can be described as an open cylinder, an iterative process is used to deduce the concentration of Rn in this well-mixed air for different times during the exposure. Again, employing the technique of using a series of linear functions to describe this time-dependent Rn concentration the differential equation can again be solved.

A set of experiments was then conducted to provide an empirical determination of the modeling parameters, such as diffusion coefficients, adsorption coefficients, and diffusion barrier dimensions. The

parameters for the various detectors, both open face and diffusion barrier, were determined by first loading the canister with ^{222}Rn and then measuring the desorption from the canister into a space with low Rn concentrations over a period of a few days. These experiments were done by counting the 609 keV peak from ^{214}Bi, a radon decay product, with a 3 x 3 NaI detector in a low-background lead-shielded counting enclosure through which air was circulated.

In a second set of experiments, conducted in a chamber, several canisters of each type were placed in the two rooms of the chamber. One room had a high ^{222}Rn content, averaging between 3.5 and 7 kBq m^{-3}, and the other with a lower ^{222}Rn content, averaging between 200 and 1000 Bq m^{-3}. The actual ^{222}Rn concentrations were measured over time using continuous radon monitors. Several canisters were switched from room to room during the middle of the exposure to expose them to high-low, and low-high variations. Results of the experiment are summarized in Table 1. As can be seen from the table, comparisons between the model and the measured charcoal device concentrations are quite good, for both the open face and the diffusion barrier devices. These results also indicate that the diffusion-limited charcoal detectors do in fact integrate better than their open face counterparts.

This work has also demonstrated the limitations in using charcoal canisters to obtain integrated readings over short periods of time when the actual ^{222}Rn concentrations are changing.

PLANNED ACTIVITIES FOR FY 1988

A significant portion of the radon group research effort will be focussed on analysis of the large data set collected from the field study in New Jersey. Radon entry data will be analyzed and performance

Table 1. Response of Various Charcoal Canister Devices to Time-varying Radon Concentrations and a Comparison of Model and Measurement Results

Device	Exposure Condition*	Avg. [Rn]** (k) (1)	Charcoal Device Measured (2)	Model Prediction	|(2) - (1)| (1) (%)
Open-face Devices:					
OF#1:	H1	7.25	5.74	6.18	-21
	H1-3	5.48	3.48	3.52	-36
	H1-4	4.88	2.81	2.85	-43
	L1-4	0.81	0.34	0.30	-58
	L1,2H3,4	2.37	2.48	2.59	+5
	H1,2L3,4	3.33	0.74	0.56	-78
OF#2:	H1-4	4.88	3.29	2.52	-33
	H1,2L3,4	3.33	0.35	0.28	-90
	L1,2H3,4	2.37	2.44	2.48	+3
Diffusion Barrier Devices:					
DB#1:	H1	7.25	7.07	7.18	-3
	H1-3	5.48	5.03	5.00	-8
	L1,2H3	2.11	2.18	2.29	+4
	H1,2L3	4.37	3.37	3.59	-22
DB#2:	H1',2L3,4	2.92	2.55	2.41	-12
	L1',2H3,4	2.41	2.78	2.55	+15

* The exposure times were divided into four periods of almost the same duration. The letters H(igh) and L(ow) designate in which of the two rooms the detectors were placed. Period 1' is slightly shorter than period 1.

** Average during exposure period determined from continuous radon monitor data

of the radon reduction systems will be evaluated. Empirical models linking observed radon concentrations with parameters thought to influence radon transport will be developed. Other research will include continued investigation of the use of the NARR data set, coupled with other regional data sets on soils, house construction characteristics, etc., to provide a model for estimating regional variability in indoor radon.

Further investigation of radon transport through soils and into structures will be initiated this fiscal year. This work will consist of experimental studies of radon movement in soils using small structures with controlled leakage characteristics. In addition, the modeling of gas transport through soils will be expanded to incorporate more realistic, heterogeneous soil conditions.

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Field Surveys of Indoor Air Quality*

B.H. Turk, D.T. Grimsrud, J. Harrison, and R.J. Prill

Four field studies examining indoor air quality funded by the Bonneville Power Administration (BPA) were completed in FY 1987. The studies included (1) a comparison of new energy-efficient homes with new standard construction homes, (2) monitoring of existing single family dwellings undergoing weatherization to reduce energy consumption, (3) mitigation of excessive radon concentrations in 15 residences, and (4) a survey of 38 commercial and institutional buildings. All buildings were located in and around the Oregon cities of Portland and Salem; Spokane, Washington; and Coeur D'Alene, Idaho. Because of regulatory pressures from the Pacific Northwest Electric Power Planning Act, BPA instituted recommendations for energy conservation that have included methods for reducing the amount of outside air entering buildings. These studies examine whether concentrations of some indoor pollutants increase in response to the reduced ventilation and cause greater health-related risks.

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ACCOMPLISHMENTS DURING FY 1987

New Energy-Efficient Homes

Model Conservation Standards (MCS) for the construction of new energy-efficient houses include specifications calling for air infiltration packages leading to infiltration rates as low as 0.1 ach. These homes have air-to-air heat exchangers installed to

raise the ventilation above 0.5 ach. Twenty-nine MCS homes were monitored along with 32 new homes, built according to standard construction practices, that served as controls. The goals of the study include comparing pollutant concentrations and installed ventilation rates in the two groups of houses along with an evaluation of pollutant source strengths.

The average air leakage area measured by fan depressurization for the MCS houses was approximately 46% lower than for the Control homes. However, measured ventilation rates, determined with a passive perfluorocarbon tracer (PFT) technique are virtually identical for both groups of houses, with a geometric mean of 0.30 ach for MCS houses and 0.26 ach for Control houses, yet are still lower than the design of 0.6 ach. From the data, it is estimated that the AAHX was responsible for providing an average 0.2 ach of additional ventilation to the natural infiltration in the MCS houses.

In general, indoor concentrations of radon and formaldehyde exhibited greater dependence on the region in which a house was located than on the construction practices by which it was built. Differences in radon levels between MCS and Control houses by region or for all houses are not considered significant. Radon concentrations were higher in homes in the Spokane/Coeur d'Alene region (geometric mean 96 Bq m^{-3}) due to the local highly-permeable, gravelly soils. Portland area homes had a geometric mean of 41 Bq m^{-3}. Eleven percent of all houses in this study exceeded the BPA mitigation action level of 185 Bq m^{-3} while 16% were above the EPA guideline of 150 Bq m^{-3}. Eighteen of the 61 houses (30%) had indoor formaldehyde levels above 100 ppb, a frequently cited guideline. The combined MCS and Control houses in the Portland area had a geometric mean formaldehyde concentration of 92.8 ppb, while Spokane area homes had a geometric mean of 59.5 ppb. This difference was much greater than that between all MCS and Control homes (82 ppb vs. 72 ppb). The regional difference is likely a result of different emission characteristics of pressed-wood products used in the two areas. Indoor formaldehyde concentrations also tended to be lower in older structures suggesting that emission rates of free formaldehyde decrease as construction materials age.

Water vapor concentrations were surprisingly similar both between groups of houses and between regions, even though outdoor concentrations were considerably higher in the Portland area. Average indoor concentrations ranged only from a low of 6.29 g/Kg in Spokane area MCS houses to a high of 6.81 g/Kg in Portland area MCS houses. Control house group averages were between these extremes. Water vapor levels in Control house bedrooms were significantly higher than in other locations in these homes. There were no significant spatial differences in the water vapor concentrations in the MCS houses, presumably due to the more uniform distribution of ventilation air by the AAHX.

Existing Homes

One hundred existing homes built prior to 1980 were tested and screened for HCHO, H_2O, and Rn using mailed passive samplers. Sixteen other homes were screened only for radon during a 30 minute visit by a technician using a continuous radon monitor. Forty eight of these homes with measurable levels of HCHO or Rn were then selected for more intensive monitoring to evaluate the effects of house tightening weatherization retrofits on the concentrations of these indoor air pollutants.

In the Phase I screening sample, 45 homes were located in the Spokane, WA-Coeur D'Alene, ID area and 71 homes were located north of Portland in Vancouver, WA. The majority of these homes had pollutant levels below most currently recommended guidelines and standards. Only one newly remodeled home had HCHO concentrations above 100 ppb (136 ppb), while 98% of the homes were below 80 ppb and the total group had a mean of 36 ppb.

The mean water vapor concentration was 6.15 gKg^{-1}, very similar to that measured in the new home study. Radon, however, appears to be a pollutant of concern in the Spokane River Valley area of Washington and Rathdrum Prarie of Idaho. The average heating season concentration for 46 new and existing homes in this area is 490 Bq m^{-3} Approximately 43% of these residences had concentrations above 300 Bq m^{-3}, the National Council on Radiation Protection and Measurements guideline. Concentrations were monitored in 14 of the 46 homes over the summer using passive samplers and were observed to decline by factors of up to 16 from heating season values. An examination of soils, domestic water supplies, and building materials strongly suggests that the high concentrations are due to the local subsurface soil composition and structure.

The more intensive monitoring of the 48 homes to be weatherized in Phase II began in December. In each home, equipment was installed to monitor temperatures, windspeed and direction, and radon concentrations continuously. Passive monitors for pollutants and ventilation were also deployed along with instruments for making time-weighted average measurements of carbon monoxide (CO) and respir-

able suspended particles (RSP). This equipment was operated for a 7-10 day period before and after each stage of weatherization, which could have included wall insulation and "house doctoring" along with caulking, weatherstripping and storm windows.

Analyses of measurements show that the standard BPA weatherization package reduced the leakage in the forty houses by approximately 12 percent while wall insulation had no measurable effect. House doctoring, an intensive weatherization technique, reduced leakage another 26%.

Preliminary examination of the pollutant concentration measurements reveals that concentrations of water vapor and formaldehyde increased following weatherization by 17 and 4 percent, respectively, while radon decreased by 18%. These results will change when adjustments are made for corresponding changes that were seen in the concentrations measured in the eight control houses during the course of the study.

Detailed analysis of the results of the study continues in FY88.

Radon Mitigation

As part of a series of surveys of the effects of weatherization on indoor air quality in the Pacific Northwest, radon concentrations were measured in 46 residential buildings in the Spokane River Valley in eastern Washington and northern Idaho. Approximately 57% of these homes exceeded the 185 Bq m^{-3} guideline established by the Bonneville Power Administration (BPA) for remedial action. The average in these 46 residences was 490 Bq m^{-3}. Fifteen of these homes were subsequently selected for research on remedial techniques, with the objectives of evaluating several possible mitigation measures and of reducing the long-term average radon concentration during the heating season to below 185 Bq m^{-3} in each house.

A number of diagnostic procedures were utilized to assist in identifying the likely radon entry locations. Because pressure-driven flow of radon-bearing soil gas is generally thought to be the predominant source of radon in houses with elevated indoor concentrations, several procedures were directed toward this source.

Continuous monitoring of indoor radon concentrations, indoor and outdoor temperatures, and wind speed and direction was established in each home to provide data on premitigation baseline conditions as well as provide a means of evaluating the radon mitigation systems. In addition, seven-day-average ventilation rates were measured at the same time, using the passive perfluorocarbon tracer (PFT) technique. Local meteorological data on winds, precipitation and barometric pressure were obtained from the National Weather Service.

Several mitigation techniques were evaluated in the course of the study. Heat-recovery ventilation (an air-to-air heat exchanger, or AAHX) was employed in three houses; in two of these systems ventilation air was supplied and exhausted from the basement respectively. Reductions of about 60, 67, and 75% were achieved. In general, the AAHX units were sized to add about 1 ach of ventilation. Since the units, when properly balanced, have a neutral effect on the pressure distribution across the building shell, the radon source strength should not be affected and the radon concentration should therefore be related inversely to the ventilation rate. Use of an AAHX to control radon appears to be best suited for those cases where initial indoor concentrations are not excessive ($<$750 to 1500 Bq m^{-3}) and/or where the initial building ventilation rate is low.

Subsurface ventilation (SSV) systems were implemented in five homes, in a variety of configurations. In general, the systems consisted of 7.5 cm diameter PVC pipes inserted in one or more (up to four) locations through the basement floor slab, or in one case, ESP119, along the exterior of the foundation wall, to a point below the wall footer. The pipes end approximately 30 cm below the floor in a 60 cm diameter dry sump 60 cm deep, backfilled with clean gravel. For the interior systems, the pipes are routed either singly or in a manifold through the top of the basement to the outside of the house. Here, the pipes are connected to a centrifugal blower, sized to develop more than 125 Pa at more than 25 L/s flow.

The effects of SSV operated in a depressurization mode were dramatic for four of the five houses, with almost all configurations leading to concentrations below the 185 Bq m^{-3} guideline adopted by BPA. In three of the five houses, the SSV system was used to pressurize the soil below the slab. In all three cases, the first floor radon concentrations dropped further. In house ESP111, subsurface depressurization resulted in a factor of two reduction in first floor radon concentration, while subsurface depressurization produced a concentration reduction of more than a factor of 10 over baseline conditions. It appears that in highly permeable soils, characteristic of this region, pressurization of the soil below the basement slab dilutes the soil-gas radon concentrations. Thus, even though the pressure differential across the building substructure is increased somewhat by the sub-slab pressurization, the soil gas that enters has a reduced radon concentration. This sys-

tem requires further study, particularly in situations were the soil permeabilities are lower than in the Spokane River Valley.

Basement overpressurization was used for four homes. The basements in each home were first sealed, including leakage paths between the basement and first floor. The basements were pressurized with a 100 - 200 L/s fan, using heated air from the first floor. This technique caused first-floor radon concentrations to be reduced below 185 Bq m^{-3}.

Basement pressurization and subslab ventilation were compared in one house, ESP120. This particular house had stone basement walls and a partially finished basement. The substructure leakage area was large; an estimated 20 percent of the total air infiltration into the house was soil gas, resulting in the relatively high indoor radon concentrations observed. This large substructure leakage may help explain why basement pressurization was somewhat more successful than subsurface ventilation.

Sealing techniques, by themselves, yielded only slight reductions in indoor radon concentrations, due in part, to the difficulty in gaining access to all the wall and floor surfaces in finished basements. Sealing the membrane between the crawlspace and the first floor produced modest reductions in first floor radon concentrations. Ventilation of the crawlspace areas also helped reduce radon levels. With the addition of mechanical ventilation to the crawlspace in one house, further radon concentration reductions were observed.

Commercial and Institutional Buildings

A survey of 38 commercial and institutional buildings involved monitoring of ventilation rates and indoor air pollutant concentrations. The objectives were to (1) inventory these parameters in non-residential, non-industrial facilities, (2) furnish data to assist in establishing energy conservation and ventilation guidelines and, (3) examine relationships between indoor air quality and ventilation rates. Pollutants monitored included formaldehyde, water vapor, radon, nitrogen dioxide, respirable suspended particles, polycyclic aromatic hydrocarbons, carbon dioxide, and carbon monoxide. Neither volatile organic compounds (other than formaldehyde) nor airborne microorganisms were monitored in this study because of budget limitations. Two buildings were monitored twice for a total of 40 building assessments. Buildings ranged in age from 6 months to 90 years, in size from, 28 to 34,000 m^2, and in occupancy from 25 to 2500 people. From 6 to 20 pollutant sampling sites were located in each building during the two week (10 working day) monitoring period. Sampling was started at the beginning of each working day and stopped at the end of occupancy for an accumulated minimum of 75 hours. Selected RSP filters were analyzed for up to 16 polycylic aromatic hydrocarbons (PAH) including benzo(a)pyrene (BaP). Carbon dioxide (CO_2) was monitored at up to two locations for a one day period, while CO was sampled at up to seven locations for one 7-10 hour day. Twice daily observations of the ventilation system were recorded for use during a later tracer decay ventilation test. Data were also collected that describe building construction, materials, occupancy, smoking policies, and activities. Ventilation rates were measured in all buildings with a one time tracer dilution and decay test conducted over one 12-hour period during unoccupied hours. The ventilation systems were set up to mimic the conditions of the two week pollutant monitoring period, while a centrally located gas chromatograph with an electron capture detector monitored the decay of sulfur hexafluoride (SF_6) at up to nine building locations.

In general, measured ventilation rates were high and pollutant concentrations were generally quite low and seldom exceeded commonly recognized standards and guidelines.

High water vapor concentrations may have caused problems of occupant comfort at sites in six buildings, most of which were monitored during higher temperature summer months.

Carbon dioxide eight-hour averages ranged from a low of 340 ppm to a high of 840 ppm with a peak 15 minute reading of 1290 ppm in one classroom. Readings rarely exceeded 800 ppm.

Only 29% of the eight-hour time-weighted average carbon monoxide measurements were above the minimum detectable level of 2 ppm.

Nitrogen dioxide levels at only two of 245 sites exceeded the EPA ambient (outdoor) annual air standard of 50 ppb. Most sites with elevated concentrations were exposed to outside air containing NO_2 from vehicular exhaust.

Of all pollutants monitored, respirable suspended particle (RSP) concentrations most frequently exceeded conservatively recognized guidelines, with occurrences usually related to nearby tobacco smoking. Building mean RSP ranged up to 67 $\mu g/m^3$. It is estimated that approximately 34% of the smoking sites in a similar sample would have RSP concentrations above the annual EPA limit of 50 $\mu g/m^3$ for suspended particles whole diameters are less than 10 μm (a larger subset of suspended particles than RSP).

Polycyclic aromatic hydrocarbon concentrations, including benzo(a)pyrene, were positively correlated to RSP concentrations and, thus, to nearby smoking

with a maximum B(a)P concentration of 9.67 ng/m^3, considerably above the U.S. ambient urban concentration of 2 ng/m^3.

Formaldehyde concentrations were quite low. The averages in only 21 buildings were above the 20 ppb detection limit. It is estimated that only 3% of all similarly selected sites would have concentrations above the ASHRAE 100 ppb guideline.

The geometric mean of all radon measurements was 20 Bq m^{-3}, similar to levels found outdoors, with only one building having concentration of concern at 290 Bq m^{-3}. The latter condition is likely due to open soil in the basement and a network of underground service tunnels allowing ready entry of the gas.

The one-time ventilation measurements from all buildings average 1.5 ach and ranged from a low of 0.2 ach to 4.1 ach. Buildings with low ventilation rates were not usually associated with indoor air quality problems, although local ventilation (i.e., ventilation rates in specific regions or rooms) may fall below ASHRAE recommendations of 5 cfm/occupant in non-smoking areas and 20 cfm/occupant in smoking areas.

Correlation is weak between pollutant concentrations and ventilation rates (both with outside and recirculated air). This is probably due to a larger variability in source strengths between buildings than ventilation rates.

PLANNED ACTIVITIES FOR FY 1988

Analyses of data from all the projects will be completed and journal articles containing the major results of the studies will be written.

Volatile Organic Contaminants In Indoor Air*

J.M. Daisey and A.T. Hodgson

Energy conservation has become an integral part of current building practices in the U.S. Reductions in ventilation rates have been found to be a particularly cost-effective means of conserving energy. However, decreased ventilation in combination with increased uses of synthetic building materials and consumer products in new and renovated buildings have been associated with increased complaints about "sick building syndrome" and related losses of work days. Emissions of volatile organic compounds (VOC) from materials used to finish interiors of buildings are suspected to play a significant role in "sick building syndrome." The major sources of these compounds have not been fully identified nor are the factors controlling their indoor concentrations well understood.

The goals of the Indoor Organic Chemistry Group are to identify the airborne contaminants that contribute to "sick building syndrome," to identify their sources and to develop a fundamental understanding of relationships between building materials, energy-conserving construction practices and ventilation so that effective mitigation strategies can be developed. This research has targeted VOC which include irritants and carcinogens and which have been shown in previous work in this laboratory to be emitted from widely used interior building materials. In FY1987, the specific research objectives were:

1. To program the temperature and humidity controllers of the Environmental Chamber and evaluate Chamber performance;
2. To investigate relations between ventilation rate and VOC source strengths in both field and laboratory experiments;
3. To develop a conceptual framework for theoretical models to describe emission rates of VOC from interior building materials as functions of ventilation rate, material age, chamber temperature and mixing and loading;
4. To investigate the effectiveness of portable air cleaners in reducing NO_2 and VOC in indoor environments;
5. To analyze the data from field experiments on personal exposures to methylene chloride from paint removers to determine exposures for various use scenarios and

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environments, to evaluate mitigation strategies and to evaluate the predictive capability of the mass-balance exposure model;

6. To determine indoor concentrations of extractable organic matter and polycyclic aromatic hydrocarbons in respirable particles collected in woodburning homes in Wisconsin.

ACCOMPLISHMENTS DURING FY 1987

Environmental Chamber

The temperature and humidity controllers for the Environmental Chamber were programmed and Chamber performance was evaluated. Background decay rates for NO_2 and six VOC were found to be 0.1 h^{-1} when the Chamber was operated in static mode. Decay rates were also found to be very reproducible in duplicate Chamber experiments.

Measurements of VOC in Large Buildings

A long-term study of a new office building in Portland, OR was begun in collaboration with R. Grot of the National Bureau of Standards. The objectives of the study are: 1) to determine long-term temporal changes in source strengths of VOC over a period of a year; 2) to identify the major sources of VOC in the building; 3) to determine short-term temporal changes in the source strengths of VOC as a function of building ventilation rates; 4) to determine temporal variations in the concentrations and source strengths of VOC over one week.

The building has seven office stories with three return air shafts. The three basement levels, used as a garage, have a separate ventilation system. Occupancy of the building was begun in April, 1987 before the building was completed. The building was completely occupied by the end of August, 1987. The major interior finish materials in the building are the same on each floor. No smoking is permitted on the office floors. Continuous ventilation measurements are being made by R. Grot using SF_6. The range of ventilation rate for the building is 0.5 to 2.0 air changes per hour.

A survey of the building was completed, the major interior finish materials were inventoried and samples of VOC were collected in the building during two field experiments. Major finish materials in the building include carpet tiles, carpet spray adhesive, rubber tile floor and adhesive in the stairwells, vinyl base cove and adhesive, painted gypsum board walls, office furniture and partitions. The VOC samples were analyzed by gas chromatography-mass spectrometry (GC-MS) to identify and quantify individual VOC. A portion of each sample was also analyzed for total hydrocarbons (THC > C_4) using a flame ionization detector with no chromatographic separation. Twenty-three individual compounds, C_9 through C_{12} aliphatic hydrocarbons, were identified.

The sums of the concentrations of the individual VOC in the building, which were quantified with GS-MS, averaged approximately 0.5 mg-m^{-3} in both August and October. By comparison, the average concentrations of the THC were about ten to twenty times higher. The latter measure includes many branched-chain hydrocarbons for which analytical standards are not available and which therefore cannot be individually quantitated. The concentrations of the THC, which were 4-10 mg-m^{-3}, are in the range in which irritant effects have been observed in subjects exposed to a synthetic mixture of 20 VOC in a chamber.[1] Some of the compounds in that mixture were present in the Portland building, although at lower individual concentrations. Specific source strengths for the sum of the individual VOC and for THC, were calculated from a single-equation mass-balance model. Based on the THC concentrations, the specific source strengths for the building were in excess of 4 mg-kg^{-1}-h^{-1}. No significant change in specific source stengths was observed between August and October.

Development of Models

Previous work in this laboratory showed that a six-fold increase in the ventilation rates in two large buildings decreased the concentrations of VOC by only one-half to one-third.[2] It was hypothesized that the emission rates of VOC were dependent upon the concentration gradient between the source and the indoor air as a driving force. This effect was also noted in small chamber measurements of VOC emissions from an assemblage of carpet and carpet adhesive. There is a need to develop quantitative models for this phenomenon so that the effects of ventilation changes can be reliably predicted and so that emissions measurements in small chambers can be reconciled with those made in large chambers and in buildings. An understanding of this effect is also important for the development of standard methods of measuring emissions rates. During FY 1987, a conceptual framework for a model was developed in collaboration with M. Sherman. The effective ventilation concept developed by Sherman and Wilson, will provide the basis of the model.[3] Experiments were designed to determine whether material bulk

resistance or air resistance dominate the rate of emissions of VOC from a given material. The base cove or carpet adhesive from the Portland building will be used for the planned experiments.

Efficiencies of Portable Air Cleaners for the Removal of NO_2 and VOC

An increased public awareness of indoor air pollution has resulted in the development of a substantial market for portable air cleaners for use in residences and offices. Portable air cleaners are designed primarily for removal of suspended particles such as pollen and tobacco smoke. Recently, some manufacturers have claimed that their devices also remove gaseous pollutants such as oxides of nitrogen and sulfur and VOC. There is, however, little information available to consumers on the performance of these devices, other than that provided by the manufacturers.

A study was undertaken to determine if portable air cleaners, equipped with charcoal filters, have any efficacy for the removal of NO_2 and VOC at concentrations similar to those found in buildings. Experiments were conducted with four portable air cleaners using the 20-m^3 Environmental Chamber operated in static mode. For each air cleaner, the Chamber was spiked with NO_2 and a mixture of six VOC. The air cleaner was operated in the chamber for several hours. The concentration of NO_2 was continuously monitored and samples for subsequent analysis of VOC were periodically collected. Decay rates due to operation of the air cleaner were calculated as the difference between the decay rates in the Chamber with the air cleaner in operation and the Chamber background decay rate.

Table 1 presents the effective cleaning rates (ECR) for the VOC and NO_2. This is the product of the removal rate times the volume of the Chamber (20 m^3) and provides a measure of the effective volume of air from which NO_2 and VOC are removed by the air cleaner in one hour. This measure is useful for evaluating the effects of air cleaners in rooms of different sizes or for comparing air cleaning to ventilation as an indoor air quality control technique. Duplicate experiments were conducted with the Air Cleaner D to assess experimental variability. The same filter was used in both experiments.

There were substantial variations among the air cleaners with respect to the ECR for NO_2 and VOC. For Air Cleaners A and D, the ECR ranged from 31 to 51 m^3-h^{-1} for five of the VOC. The ECR for NO_2 averaged 75 m^3-h^{-1} for Air Cleaner D and 42 m^3-h^{-1} for Air Cleaner A. Since Air Cleaners B and C had very low ECRs, they have very little utility as control devices for NO_2 and VOC.

The ECR for NO_2 decreased from 79 to 71 m^3h^{-1} in the second experiment with Air Cleaner D. This difference was statistically significant ($p=0.01$). The ECR for the n-heptane, 2-butanone and toluene were also lower and significantly different ($p \leq 0.05$) in the second experiment. Differences in ECRs for the remaining VOC were not significantly different.

Of the three air cleaners, Unit D had the highest removal rate for NO_2. Unit B had the lowest removal rate for NO_2, which was only about 2.5 times greater than the background decay rate. None of the air cleaners effectively removed dichloromethane, an organic solvent commonly used in paint removers and other consumer products. The vapor pressure of this compound at 25°C is 427 mm and is four times higher than that of the compound with the

Table 1. Effective Cleaning Rates for NO_2 and VOC.

	Effective Cleaning Rate (m^3h^{-1} ± 95% C.I.)				
				D	
Compound	A	B	C	Exp 1	Exp 2
NO_2	42 ± 1	5.14 ± 0.08	6.2 ± 0.2	79 ± 1	71 ± 2
Dichloromethane	2 ± 1	0	0	0	0
2-Butanone	31 ± 4	0	8 ± 2	49 ± 13	37 ± 4
n-Heptane	47 ± 1	3.1 ± 0.6	18 ± 1	51 ± 2	41 ± 3
Toluene	43 ± 3	3.2 ± 0.6	17 ± 1	45 ± 2	41 ± 2
Tetrachloro-ethylene	41 ± 2	2.5 ± 0.6	14 ± 1	44 ± 2	41 ± 2
Hexanal	37 ± 6	4.6 ± 0.9	10	39 ± 6	18 ± 4

next highest vapor pressure, 2-butanone (95.5 mm). Air Cleaners A and D both had ECRs for the remaining VOC of about 40 m^3-h^{-1}. These two devices operate at high flow rates and incorporate relatively large amounts of charcoal. Air Cleaner B did not remove 2-butanone and had low removal rates for the remaining VOC.

Exposures to VOC from Use of Consumer Products

Usage of consumer products in buildings and residences can be a major source of VOC in indoor air. High exposures to methylene chloride (CH_2Cl_2) from the use of paint removers and aerosol finishes are of particular concern since this compound is metabolized to CO leading to elevated levels of carboxyhemoglobin and possible anoxic stress. In addition, this compound has recently been reported to be a carcinogen in animals.

Source strengths and personal exposures to CH_2Cl_2 were previously characterized in the Environmental Chamber at two ventilation rates for typical applications of paint removers and aerosol finishes.[4] This investigation was extended in 1987 to include field measurements of personal exposures to CH_2Cl_2 from paint removers in residential environments for a variety of use scenarios.[5] The objectives of the field measurements were to identify practical ways to minimize personal exposures resulting from the use of paint removers and to evaluate the mass-balance model previously developed for predicting exposures in the residential environment.

A total of 21 experiments were conducted outdoors and indoors in a garage, a basement workshop, and in large and small rooms of a house. In the work areas, ventilation patterns and rates were varied by opening windows and doors and by the use of a household fan. Finishes were removed from uniformly-prepared panels or from chairs. The personal exposure of the worker was determined by continuous measurement of CH_2Cl_2 in a pumped breathing zone sample.

Personal exposures resulting from the outdoor use of paint remover were very low (6-36 ppm-h). Exposures from the use of paint removers indoors without mechanical exhaust ventilation were considerably higher, 190 to 2090 ppm-h. In each indoor location, an open window or exterior door reduced exposures by one-half relative to the closed condition. Exposures were greatly reduced by a fan placed near the work area, exhausting through an open window (11-142 ppm-h).

A single-equation mass-balance model was used to produce estimates of theoretical exposures for experiments conducted indoors. The efficacy of the model for predicting exposures was evaluated by comparing the theoretical and measured personal exposures. The model performed best for small-volume work areas with low ventilation rates. In general, the model had an accuracy of ± 50 percent when applied to experiments conducted in enclosed work areas without an exhaust fan.

Effects of Woodburning Stoves on Indoor Air Quality

Deterioration of outdoor air quality due to residential woodburning has been widely documented. To date, most studies of indoor air pollution have focused on total or respirable particulate matter concentrations and have sought to assess the impact of woodburning stoves on indoor air quality by comparing indoor and outdoor levels. In a pilot study, the effects of woodburning on indoor particulate air pollutants were examined by comparing air quality during woodburning and non-woodburning periods. Concentrations of respirable particulate matter (RSP) (D_{50}=3.5um), dichloromethane-soluble (DCM) and acetone-soluble (ACE) particulate organic matter and eight polycyclic aromatic hydrocarbons (PAH) were compared in seven Wisconsin homes.[6]

There were no significant differences between RSP concentrations during the woodburning and non-woodburning periods. Concentrations of the total organic-soluble matter (DCM plus ACE), however, averaged 10.4 $\mu g/m^{-3}$ during woodburning periods which was approximately twice the average concentration during non-woodburning periods. The concentrations of total measured PAH were 2 to 46 times higher when the woodstoves were in operation. The source strength for the sum of the DCM plus ACE fractions was estimated to be 1.5 mg-h^{-1}. This is consistent with the range of the source strengths of total particulate matter reported for airtight woodburning stoves.[7]

Soil-Gas Transport: A Mechanism of Indoor VOC Exposure

Human exposures to toxic VOC from hazardous waste sites can occur through several routes. Most investigations have focused on exposures which occur through ingestion of contaminated water or inhalation of outdoor air contaminated by releases of VOC from such sites. Another potentially significant exposure pathway is pressure-driven flow of VOC

contaminated soil gas into building substructures and the subsequent distribution of VOC throughout the building. This flow is driven by the pressure gradient established across the building substructure and soil by thermal differences between indoors and outdoors, by wind loading on the building superstructure, and, in some instances, by the operation of mechanical systems (e.g., unbalanced exhaust ventilation).

Evidence of the importance of this pathway is provided by work at LBL that has shown that this is the major pathway of exposure for radon, but there has been almost no research on the significance of this pathway for VOC. In the fall of 1987, field experiments were conducted at a house with a full basement located near a landfill in California. The objectives of these experiments were: 1) to determine the identities and concentrations of VOC in soil gas, indoor and outdoor air and well water at the site; 2) to measure source strengths for VOC entering the house by gas-phase migration through the soil; and 3) to measure the source strengths of VOC due to the use of heated well water for showers.

The field experiments were completed and all samples have been analyzed for VOC. The data from the field experiments are now being analyzed. Some preliminary results, however, are available. The major VOC identified in the soil gas and well water were Freons 11 and 12, tetrachloroethylene, and 1,1,1-trichloroethane. These compounds were also found in the house. Source strengths of these compounds increased in the basement as the house was depressurized, supporting the hypothesis that VOC can be transported into a building by this mechanism. Exposures to the VOC from soil-gas transport will be compared to those from uses of VOC-contaminated water.

PLANNED ACTIVITIES FOR FY 1988

- Complete field experiments on the spatial and temporal variations in source strengths of VOC in the Portland office building and begin to analyze the data with respect to ventilation rate.
- Conduct Chamber experiments on emissions of VOC from building materials.
- Continue work on the development of models for the mass transport of VOC from building materials and for source identification of indoor air pollutants.
- Prepare a paper on the results of the pilot study on a tracer method for sources of indoor particulate matter.
- Complete Chamber experiments on the portable air cleaners; prepare a report and a paper on the results of the experiments.
- Analyze the results of the field experiments on pressure- driven flow of VOC-contaminated soil-gas; prepare a report and a paper on the results.
- Conduct pilot studies of the heterogeneous reactions of NO_2 on interior materials found in buildings.
- Serve as a member of the National Research Council's Committee on Advances in Assessing Human Exposures to Airborne Pollutants.

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Indoor Exposure Assessment*

G.W. Traynor, A.V. Nero, S.R. Brown, J.C. Aceti, M.A. Apte, J. McCann, and B.V. Smith

The Indoor Exposure Assessment Project has three major research themes: 1) to continue the development of a macromodel to characterize the frequency distribution of exposures to indoor pollutants; 2) to compile a data base of field measurements of indoor pollutants; and 3) to conduct assessments of the health risks associated with exposures to indoor air pollutants. Conceptually, the first two projects supply the exposure data needed for the third project of assessing health risks from indoor air pollutants.

In FY 1987, modeling efforts assessing the distribution of indoor exposures to combustion pollutants were continued; the concentration of indoor pollutants (CIP) data base was expanded; and the overall assessment of carcinogenic risk from indoor exposures was advanced.

MACROMODEL TO ASSESS INDOOR EXPOSURE DISTRIBUTIONS

Accomplishments During FY 1987

A major effort of the Indoor Exposure Assessment Project has been to utilize available information on the behavior and occurrence of indoor pollutants as a basis for assessing, in a systematic way, the distribution of public exposures to important classes of indoor pollutants. An important manifestation of this effort has been the development of elements of a model that calculates such exposure distributions, based on mass-balance principles and on available data on the factors affecting indoor concentrations. Initial efforts of the project focussed on the problem of estimating exposures to combustion emissions, and these efforts have expanded with the participation of other contractors supported by the Department of Energy's Office of Environmental Analysis. (These were K. Novak at Brookhaven National Laboratory, L. Green at Mueller Associates, Inc., and A. Smith-Reiser at Energetics, Inc.).

Many previous efforts have focused on specific aspects of indoor air pollution due to combustion sources.[2] However, there does not exist a cohesive model that can characterize the distribution of indoor combustion pollutant concentrations in residences on a regional, national, temporal, and/or source basis. It is the goal of this project to develop, calibrate and verify such a distributional model, initially for combustion emissions, then for other pollutant classes. Such a model will be a useful tool to 1) quantify the impact of combustion sources on indoor air quality (IAQ), 2) identify high-risk populations exposed to high indoor pollutant concentrations, 3) direct policy decisions regarding energy conservation, new housing codes, and source emission rates, 4) identify key parameters to target for control/mitigation efforts, 5) assist in the quantification of pollutant exposures for epidemiology studies, and 6) direct data collection efforts of future national/regional IAQ field studies.

The model is based on, and is an expansion of, mass balance principles commonly used in IAQ studies. Keys to the model include the characterization of building stock parameters relevant to IAQ (e.g., house volume, air exchange rate), the investigation of the market penetration of combustion appliances and other indoor combustion sources, and the development of source usage models. The macromodel takes advantage of existing laboratory and field research on appliance pollutant emission rates and pollutant-specific building penetration factors and reactivity rates. The model also utilizes existing

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regional and national data (from utilities, state agencies, federal agencies and trade organizations), when available, for model inputs. The model utilizes deterministic and Monte Carlo simulation techniques to combine all of the inputs yielding indoor pollutant concentration distributions.

The first phase of this project is to develop the model from mass balance principles and incorporate existing data into the model. Initial efforts in the development phase focus on carbon monoxide (CO), nitrogen dioxide (NO_2), and respirable suspended particle (RSP) levels in single-family residences.

The second phase of this project is to calibrate the model. Calibration can take two forms. First, the equations in the model may need adjusting or expanding based on field studies designed to test one or more parts of the model. For example, the equation describing the usage of primary space heating appliances may need modification based on a field study designed to test that part of the model. This first type of calibration can be considered to fall under the general category of model improvements. This second type of calibration activities fall under the general category of data improvement. For example, a field study designed to measure the pollutant emission rate distribution of gas wall furnaces would provide additional information to calibrate the model. Sensitivity analyses will be used to rank the relative importance of various information gaps to efficiently guide calibration efforts involving field studies.

The final phase of the project is to conduct a verification of the entire model by comparison wit data developed over a period of years. Although specific aspects of the model will have been tested as part of the calibration efforts, the complete model will still need validating in order to establish its adequacy for the purposes intended.

Although the initial modeling efforts concentrate on three combustion pollutants, the model is being developed with explicit attention to future expansion of the model to describe other indoor air pollutants concentrations from a wide variety of sources.

This effort is essentially an expansion of previously published ideas directed at efficiently utilizing monitoring and modeling efforts to understand the indoor combustion-related air pollution picture[3,4]. The indoor pollutant concentration distributions developed as part of this study can be combined with activity patterns to assess residential exposures to combustion pollutants. Exposure to residential indoor pollutants is part, often the dominant part, of a person's total exposure[5].

Preliminary modeling and data collection efforts have identified several information gaps that need to be filled. An important information gap is the distribution of venting factors for partially vented appliances such as wood stoves and malfunctioning vented appliances. Other information gaps include appliance (or source) usage rates and some pollutant emission rates. Although the pollutant emission rates of several combustion appliances have been tested in the laboratory, field studies need to be conducted to verify or modify the laboratory results. Different appliance types, ages, and models and different frequencies of maintenance can cause appliances in the field to have different pollutant emission characteristics than the few appliances that have been tested under laboratory conditions. Numerous other, yet less significant, information gaps have also been identified.

The preliminary modeling results do support many intuitive notions regarding populations exposed to the highest indoor pollutant concentrations. High indoor CO concentrations are associated with poorly tuned unvented gas or kerosene space heaters, malfunctioning vented appliances, and leaky wood stoves. High indoor NO_2 concentrations are associated with unvented gas or kerosene space heaters and malfunctioning vented appliances. High indoor RSP concentrations are associated with leaky wood stoves and indoor cigarette smoking. Houses with multiple combustion-pollutant sources with independent source usage patterns, such as houses with leaky wood stoves and cigarette smokers, have the highest indoor pollutant levels. Houses with only gas cooking ranges are not associated with relatively high indoor pollutant concentrations unless they are used to heat the house or are maltuned.

Planned Activities for FY 1988

The planned activities for FY 88 are: 1) complete the initial development of the model to assess indoor exposure to combustion-generated pollutants; 2) conduct sensitivity analyses and micro/macro comparisons of the model to rank information/modeling gaps; and 3) explore the potential for generalizing the model and expanding it to include combustion pollutants other than CO, NO_2, and RSP (e.g., polycyclic aromatic hydrocarbons, dinitropyrenes or other organic mutagens), radon, and non-combustion organic contaminants such as those arising from building materials, furniture, and consumer products.

CONCENTRATIONS OF INDOOR POLLUTANTS (CIP) DATA BASE

During the last ten years public and governmental concern regarding indoor air quality in this coun-

try and elsewhere has greatly increased. This concern has resulted in hundreds of field experiments being carried out to monitor pollutant concentrations and other relevant parameters in a wide variety of building types and geographic locations.

The results of this research have been published in a variety of different journals, conference proceedings, and reports. This diversity of source material, combined with the rapid growth in the amount of research being carried out, has made it apparent that a centralized collection of these data in an easily accessible form would facilitate the transfer and distribution of knowledge regarding indoor quality, both within the research community and to other involved entities, such as architects, builders and energy utilities.

The goal of this project is to create a computerized data base of the results of field studies devoted to monitoring indoor air quality in occupied buildings in the United States and Canada.

Accomplishments During FY 1987

A major update to the Data Base was prepared during FY 87. Seventy-four new bibliographic references were added, and forty-one new summary data sets. Several minor enhancements to the software were made, including the ability to output data to a text file as well as to a screen and printer.

Software was written to support user entry and editing of summary search data. When distributed, this would make it possible for the user to enter not only their own bibliographic data, but also summary data and text.

The first draft of a technical reference manual was prepared. This manual is designed to provide a journeyman programmer with enough information to modify and extend the data base system. It includes file specifications, heavily commented source code, a subroutine tree, and other useful information.

The CIP Data Base (Version 3.1) has been implemented in a microcomputer environment running MS-DOS, using dBase III, and a commercial dBase III compiler, Clipper. Copies of the CIP Data Base are distributed on floppy diskettes to individuals for their own use, avoiding the time-sharing and phone charges of mainframe data bases, and allowing customization and additional data entry by the user. Periodic updates to the data base are distributed to users, also on floppy diskettes. The system is shipped to the user on 7 floppy diskettes, together with a 45-page user manual, and a printout of the bibliographic database in a 3-ring binder. User support is provided both over the phone by project staff and via a periodic newsletter distributed to all users. Updates to maintain the currency of the data base are distributed 1-2 times a year.

The CIP Data Base is a stand-alone system, with menu-driven functions and on-line help to facilitate entry, retrieval, and searching. Both bibliographic information and summary text and data are retrievable. Some of the available search parameters are author, pollutant range, title, keyword, year of publication, geographic region, country, state or province, building type, building material, instrumentation used, sampling method used, climate, and ventilation system and rate.

The CIP Data Base organizes reports of experimental work into two components, a bibliographic data base and a data base of summary data and text. Each has its own structure, search, and retrieval/display capabilities. Below is a brief specification of the system:

Required Microcomputer: IBM PC/XT/AT,
or a compatible
Language: compiled dBase III using Clipper
(Nantucket Software)
Operating system: MS-DOS & PC-DOS,
Version 2.0 or later
Minimum Hardware configuration required:
1 Floppy disk drive and
1 Hard disk drive
Required Memory: 352 Kbytes
User training required: Minimal
Documentation: On-line/interactive + extensive
external documentation
Data structures: 8 database files, 4 permanent,
4 temporary; 7 indexes, 6 permanent,
1 temporary; 1 ASCII text file
per summary dataset.

Planned Activities for FY 1988

Additional updates to the data base will be distributed during the fiscal year. The updates will include published work and final reports through June or July, 1988, and will, in particular, include the papers from the International IAQ conference in Berlin 1987. In addition, the user community will continue to be supported. There are 200 current users of the CIP Data Base.

RISK ASSESSMENT

The purpose of this work is to utilize exposure information as a basis for estimating the health risks due to various classes of indoor pollutants.

Accomplishments During FY 1987

Earlier work in this area has made sufficient progress in examining risks of major pollutant classes that, together with other information, it is now possible to assemble tentative pictures of risk for certain health endpoints, at least for diseases like lung cancer, that are usually fatal.

The LBL effort has previously examined data on indoor radon concentrations as a basis for estimating the distribution of indoor concentrations, and hence exposures, in U.S. homes.[6] This indicates that the average indoor concentration is approximately 1.5 pCi/l (55 Bq/m^3) in single-family homes and that approximately 7% (or 4 million houses) have annual-average concentrations exceeding 4 pCi/l (150 Bq/m^3). Together with various epidemiological data, this leads to an estimate of the average lifetime risk of lung cancer due to radon exposures of about 0.4%,[7] with long-term occupants of houses with 150 Bq/m^3 incurring a risk exceeding 1% and those living at higher concentrations having proportionately higher risks.

This defines a spectrum of risk from radon (see Figure 1) that is much higher than the risks associated with typical environmental pollutants, i.e., those in outdoor air and in water supplies, and that compares with occupational risks or with risks associated with personal choices - e.g., accidents in homes or cars or, in the extreme, cigarette smoking. Similarly, analysis of organic chemicals indoors leads to an

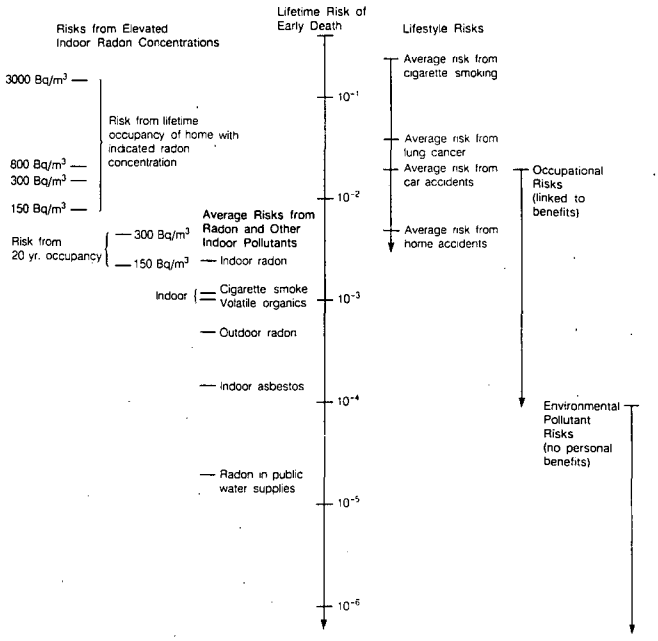

Figure 1. Comparison of risk of premature death for various exposures and settings. (XBL 871-9909B)

estimated average risk of cancer of 0.03-1% due to indoor exposures (depending on the form of dose-response model used).[8,9] This again is a large risk compared with other environmental situations.

This picture of risk of premature death due to indoor exposures can be filled out by noting the estimated effects of two other pollutants about which there has been much concern: environmental tobacco smoke (ETS) and asbestos.[10] Although controversial, midrange estimates of the risk of lung cancer to the average nonsmoker, due to breathing ETS, is comparable to the middle of the estimated range for organic chemicals just noted. Estimates of the risk from asbestos exposure, arising primarily indoors, are somewhat lower. Nonetheless, estimated risks from all of these indoor pollutants just named exceed 10^{-4}, which is larger than most environmental risks. This more complete, albeit tentative, picture of the risks of indoor pollutants provides a direct basis for considering the importance of indoor pollutants and influences the design of strategies to control indoor air pollution levels by contributing to fuller development of our general perspective on risks due to pollutant exposures.

Planned Activities for FY 1988

We will 1) reexamine radon risk estimates in the light of new data on U.S. radon concentrations and reanalysis of the full body of epideiological data, 2) undertake a general evaluation of our current state of knowledge on organic chemicals and their importance, and 3) begin to include results from combustion exposure modeling in assessment of indoor risks.

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Ventilation and Indoor Air Quality Control*

W.J. Fisk, P.H. Wallman, R.J. Prill, R.J. Mowris, and D.T. Grimsrud

The Ventilation and Indoor Air Quality Control Project conducts research on techniques for limiting the concentrations of pollutants in indoor air - these include methods of ventilation, air cleaning, and minimizing pollutant source strengths. Objectives are to evaluate existing and proposed technologies and to develop new technologies. Evaluation criteria include the influence of a technology on indoor pollutant concentrations, the associated energy requirements or savings, and costs. Research is performed through a combination of laboratory experiments, field studies, modeling, and analysis of the work performed by others.

During FY 1987, project staff focused on the following four efforts: 1) a laboratory evaluation of exhaust-air heat pump performance; 2) modeling the influence of different residential ventilation techniques on indoor radon; 3) a laboratory study of thermal decomposition of tracer gases; and 4) detailed field studies of ventilation within commercial buildings. Summaries of activities in the four areas are provided below.

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ACCOMPLISHMENTS DURING FY 1987

Exhaust Air Heat Pumps

In a residential mechanical ventilation technique that is being introduced in the United States, an exhaust fan draws air from various indoor locations at a controlled rate. This air is blown through the evaporator of a small exhaust-air heat pump (EAHP) and is then exhausted to outside. Makeup air is drawn into the building through unplanned cracks and holes and, optionally, through adjustable-size, strategically-placed slot ventilators installed in the exterior walls. The EAHP extracts heat from the exhaust airstream and transfers this heat, plus the energy consumed by the heat pump's compressor, to the domestic hot water. Some EAHPs contain a fan coil (i.e., either a second condenser or a hot water coil plus a fan) so that heat can also be delivered to the indoor air, reducing the load on the furnace system.

During FY 1985 and FY 1986, we developed and utilized a computer model to evaluate this ventilation technology.[1,2] During FY 1987, we completed

laboratory evaluations[3] of two EAHP systems that are now (with some modifications) being marketed in North America. System performance was monitored over a wide range of operating conditions. One of the systems (Unit A) was evaluated with and without operation of a fan-coil condenser. In the following discussion, we consider only the results of evaluations of Unit A.

The experimental results indicate that the coefficient of performance (COP) of Unit A, when used to heat water, can be correlated linearly to the average temperature of water in its tank. This correlation, which holds for a wide range of hot water demand volumes and schedules, reflects the configuration of the condenser which wraps around almost the entire vertical cylindrical surface of the water tank. When Unit A was operated with its fan coil condenser, its COP varied linearly with the temperature of air entering the fan coil.

Based on the data, simple empirical models of EAHP performance were developed. The COP of Unit A, when used to heat water (COP_w) is described by the relation

$$COP_w = -0.077\,\bar{T}_{tank} + \begin{cases} 6.55 & \text{for } R_{ex}=150 \\ 6.67 & \text{for } R_{ex}=200 \\ 7.00 & \text{for } R_{ex}=300 \end{cases} \quad (1)$$

where: $\bar{T}_{tank}$ is the average (in space and time) temperature of water within the tank (°C), R_{ex} is the exhaust air flow rate (kg/h), and the temperature and relative humidity of the air entering the evaporator, are 21 °C and 50%, respectively. The COP can also be correlated to the more commonly utilized hot water delivery temperature (i.e., the temperature of water at the top of the hot water tank), since this temperature is approximately a constant 5.5 °C greater than $\bar{T}_{tank}$. When Unit A is operated with its fan-coil condenser to heat air, its COP can be characterized by the expression

$$COP_{FC} = -0.073\,T_{in} + \begin{cases} 4.14 & \text{for } R_{FC}=200 \\ 4.64 & \text{for } R_{FC}=300 \\ 5.04 & \text{for } R_{FC}=400 \end{cases} \quad (2)$$

where: T_{in} is the temperature of air entering the fan coil (°C) and R_{FC} is the flow rate of air through the fan coil (kg/h). Finally, when both condensers are utilized (with the fan coil condenser used only when there is no demand for water heating), the average COP (COP_{combi}) can be expressed by the relation

$$COP_{combi} = X_w\,COP_w + X_{FC}\,COP_{FC} \quad (3)$$

where: X_w and X_{FC} indicate the fraction of total operating time during which the water-heating condenser and fan-coil condenser are utilized, respectively. These correlations can be used to estimate energy savings; however, they are valid only for the range of operating conditions in our studies.[3]

Unit A has an average COP that is approximately 30% greater than the COP used in our previous modeling efforts.[1,2] Using a modified version of the TRNSYS (Transient System Simulation) Program, and this higher COP, we developed revised estimates of yearly energy savings and cost of conserved energy for EAHP systems with fan coils installed in all-electric well-insulated houses (built to a model conservation standard) located in three Pacific Northwest cities: Portland, Spokane, and Missoula. Considering the relatively large predicted energy savings of 5700 to 8090 kWh, and estimated costs of conserved energy of 3.5 to 4.6 cents/kWh which are comparable to current electricity prices, this method of ventilation appears to be fairly attractive in the Pacific Northwest. Our studies also pointed out the potential advantages of a modified EAHP control system which gives priority to fan coil operation until water temperatures fall below a certain value. With such a control system, we estimate that energy savings might be increased by 15 to 20%.

Influence of Infiltration, Balanced Ventilation and Exhaust Ventilation on Indoor Radon

Most U.S. houses are ventilated primarily by infiltration, the natural leakage of air though cracks and holes in the building envelope, which is driven by wind and indoor-outdoor temperature differences. To obtain better control of the ventilation rate and to reduce energy demands, mechanical ventilation of houses that have a more air-tight envelope (to reduce infiltration) is sometimes employed. The two common mechanical ventilation options are: 1) balanced (equal supply and exhaust) mechanical ventilation with heat recovery using an air-to-air heat exchanger, and 2) mechanical exhaust ventilation as described in the previous summary.

Models suitable for examining the influence of these three ventilation options (infiltration, balanced ventilation, and exhaust ventilation) on radon (Rn) entry rates and indoor Rn concentrations were developed primarily in FY 1986. One model applies for a house with a basement surrounded by homogeneous soil with the only penetration to the soil being a wall-floor gap at the junction of the basement floor and walls. The second model applies for a house with a crawl space when the crawl space has sufficient vents to outside so that air pressures

within the crawl space are not influenced by pressures within the house.

A detailed description of the models is provided elsewhere.[4,5,6] The major parameters calculated are: 1) the magnitude of the pressure difference which causes soil gas (containing Rn) to enter through the wall-floor gap, or crawl-space air (containing Rn) to enter through the floor above the crawl-space; 2) the entry rate of soil gas or crawl-space air; 3) the Rn entry rates (based on assumed values of soil gas or crawl-space Rn concentration; 4) the building ventilation rate (using an infiltration/ventilation model); and 5) the indoor Rn concentration (using a single-zone mass balance equation).

Soil gas and crawl space air can be drawn into a house due to pressures caused by wind and the stack effect, irrespective of the method of ventilation. However, the method of ventilation influences Rn entry rates for two primary reasons. First, mechanical exhaust ventilation (but not balanced mechanical ventilation) depressurizes a house slightly which increases the driving force (pressure difference) for Rn entry. Second, the tightening of a building envelope to reduce infiltration, which generally accompanies mechanical ventilation, usually includes a tightening of the floor located above the crawl space. A reduction of the leakage area in the floor inhibits the flow of crawl-space air into the house. Each of these factors is accounted for in the models.

During FY 1987, we used the models and hourly weather data for Spokane, Washington to estimate average Rn entry rates and indoor radon concentrations for the heating season (September 16-April 30) assuming that there is negligible window opening during this time period. The calculations are performed using effective leakage areas (ELAs) and mechanical ventilation rates that vary depending on the method of ventilation so that the heating-season average ventilation rate is always approximately 0.55 air changes per hour (ach).

For a house with a basement we performed calculations with a range of soil permeabilities and soil gas radon concentrations. These calculations indicate that pressure-driven entry of soil gas and, thus, Rn should not be a problem when the soil surrounding the basement has a permeability of 10^{-12} m^2 or less. Soil permeabilities in this range or lower are common - for example, clays and silts have a permeability less than 10^{-13} m^2. Thus, from the perspective of indoor Rn, any of these methods of ventilation should be acceptable if the soil has a low permeability. Even if the permeability is in the range of 10^{-11} m^2, soil gas entry and the method of ventilation should not be important unless the soil gas has an unusually high concentration of Rn. However, if the soil permeability is in the range of 10^{-10} or $10^{-9}m^2$, our calculations indicate that exhaust ventilation, compared to infiltration at the same rate, could increase average indoor Rn concentrations by a factor of approximately 1.7 and by hundreds of Bq m^{-3}. In such situations, exhaust ventilation should be avoided unless other measures are taken to reduce Rn entry.

For a house with a crawl space, calculations were performed for three different distributions of leakage area: uniformly distributed, high floor ELA, and low floor ELA. Three crawl-space Rn concentrations were also used for calculations. Based on the calculations, a large fraction of the air that enters a house can come from the crawl-space, particularly when ventilation occurs by natural infiltration. In such instances, the indoor Rn concentration will be a substantial fraction (e.g., 50% to 100%) of the crawl-space Rn concentration. Therefore, control of crawl-space Rn concentrations (usually by crawl-space ventilation) is more important than choosing a particular type or rate of ventilation for the house. The different techniques of ventilation do lead to substantially different Rn concentrations, in a house with a crawl space. Both the mechanical ventilation options, when combined with house tightening that includes reducing the ELA of the floor, lead to substantially lower indoor Rn concentrations than the traditional reliance on infiltration. Such results are expected, because with mechanical ventilation and house tightening a larger proportion of the air that enters the house will not pass through the crawl space. Balanced ventilation leads to the lowest indoor Rn concentrations - about a factor of three lower than with natural infiltration.

The models have been used to investigate the effects of varying other parameters. One particularly interesting result for a house with a basement, is a predicted increase in indoor Rn concentrations as the rate of exhaust ventilation is increased above approximately 0.5 h^{-1}.

Thermal Decomposition of Tracer Gases

Gaseous tracers, such as sulfur hexafluoride and various halocarbons are commonly injected into the air within buildings in order to measure ventilation rates and study air flow patterns. Depending on the instrumentation utilized to measure tracer gas concentrations and the specific tracer(s) selected, maximum tracer gas concentrations may be less than 100 parts per billion or as high as several hundred parts per million. Typically, one uses tracers that are essentially non-toxic (i.e., tracers that are expected to cause no adverse health effects at concentrations sub-

stantially above those encountered during the studies).

The authors previously developed a multi-tracer measurement system for detailed studies of ventilation in commercial buildings. The tracers that can be utilized with this system are sulfur hexafluoride and refrigerants 13B1, 115, 12, and 114 (SF_6, $CBrF_3$, $CClF_2CF_3$, $CClF_2$, and $CClF_2CClF_2$). Available threshold limit values (maximum average concentration for an 8-hour workday) for these tracers are 1000 to 200,000 times greater than the maximum anticipated concentrations of tracers in our experiments; therefore, no adverse health effects are expected due to exposure to these tracers. However, it is known that these tracers and similar compounds that are commonly present in indoor air can decompose when they pass through a combustion zone or are otherwise heated to a sufficiently high temperature. The halogen acids (i.e., HCl, HF, and HBr) are generally considered to be the predominate decomposition products. Some production of phosgene ($COCl_2$), carbonyl fluoride (COF_2, carbonic chloride fluoride (COClF), and free halogens (Cl_2, F_2, Br_2) have also been suggested. Because any of these potential decomposition products are considered to be highly toxic, the possibility of thermal decomposition of tracer gases is a significant concern.

Experiments were conducted to determine approximately the rates of tracer gas decomposition caused by electric and gas range-top burners. A mixture of the five tracer gases was injected into a mechanically ventilated, artificially mixed, stainless steel chamber containing the ranges. Tracer decay rates were monitored with and without range burner operation. Additional experiments were directed at the potential for decomposition when these tracers passed through a lighted cigarette - in this case our concern is with the inhalation of decomposition products by the smoker. The concentrations of tracer gas in the air surrounding a cigarette smoking machine (which smoked the cigarette) were measured and compared to the concentrations of tracer gases in the main-stream smoke which was collected in a small sample bag. The same experiment was also conducted without lighting the cigarette.

The techniques used for this study yield results with a high uncertainty but these results are still valuable given the lack of other data. More accurate and complete data could be obtained by actual monitoring of decomposition product concentrations.

Based on the experimental results, our best estimate is that an 825W electric range-top heating element caused no tracer decomposition and that a natural gas burner (~7400 kJ/h) caused all the tracer within 2.8 to 4.2 m^3 of air (depending on the tracer) to decompose during each hour of burner operation. These volumes of air correspond to 120% to 190% of the minimum amount of air required for complete combustion of the natural gas. Considering the precision of repeated experiments, we also derived estimated upper limits (i.e., probable overestimates) of the volumes of air from which tracer is decomposed each hour - these are 1.7 m^3 and 5.3 m^3 for the electric and gas burner, respectively.

In tests with burning cigarettes, we measured repeatable (in two tests) 20% to 30% lower tracer gas concentrations in the mainstream smoke than in the air surrounding the cigarette and essentially a 0% loss of tracer when the cigarette was not lighted. These 20% to 30% losses could be due entirely to tracer decomposition; however, we can not rule out losses due to sorption of the tracers on tobacco smoke aerosols.

To estimate the decomposition product concentrations that might result from tracer gas decomposition, one can utilize the estimates of decomposition rates given above, simple mass balance models for a building or room with a known ventilation rate, estimates of the extent of range burner operation or smoking, and the principle of conservation of halogen atoms. In the case of smoking, the ratio of air inhaled through cigarettes to total air breathed, approximately 0.002 if twenty cigarettes are smoked in an eight-hour period, should also be factored into the calculations. The resulting estimated decomposition product concentrations are highly dependent on the tracer gas concentration, which can range over a factor of 1000 depending on the experimental techniques. Through such calculations we concluded that use of the five tracers noted above in commercial buildings, with maximum tracer gas concentrations of 0.2 ppm for SF_6, 0.5 ppm for refrigerant 13B1, and 1.0 ppm for the other refrigerants, should not result in adverse health effects. However, we adopted procedures to minimize the possibility of accidental releases of tracer (which might result in very high tracer gas concentrations). We also consider the possible sources of thermal decomposition in each building prior to deciding whether to study the building. Since tracer gas concentrations, the actual tracers utilized, building volumes, sources of thermal decomposition, and ventilation rates vary widely, it is recommended that the hazards associated with tracer decomposition be considered on a case-by-case basis. Further studies of this issue, to reduce uncertainties, are also recommended.

Commercial Building Ventilation Studies

The approximate building-average ventilation rate has been measured by the research community in roughly 50 U.S. commercial buildings primarily by monitoring the rate of decay of a tracer gas concentration. However, it is important to obtain more detailed information on ventilation within commercial buildings - for example, to monitor: 1) ventilation rates and the related local ages of air at different locations within buildings; 2) values of ventilation effectiveness which indicate overall patterns of air flow between locations of supply and exhaust; and 3) rates of interzone air flow or mixing. These factors influence the efficiency and capability of ventilation systems in supplying and removing heat and removing pollutants and, thus, influence indoor air quality and building energy requirements.

Using recently introduced tracer gas experimental techniques and methods of processing tracer gas data [7], it is possible to obtain much of this more detailed information on commercial building ventilation. (The specific information that can be obtained depends on the building and experimental methods employed.) In prior fiscal years, we identified a group of five gases that are suitable for use as tracers and that can be monitored using one instrument, developed measurement and calibration procedures, developed and evaluated methods of tracer gas injection and sampling, and conducted tests of measurement precision and accuracy [8]. During FY 1987, multi-tracer experimental systems for use in buildings were fabricated and monitoring was completed in two buildings.

There are three major components of the experimental system. The core of the system is three cart-mounted gas chromatographic systems for measuring tracer gas concentrations; each system samples air through one to three sample lines. These cart-mounted systems are generally placed in the building mechanical room(s) and used to monitor tracer gas concentrations within the major air handling units (AHUs) - for example: the concentration in the return/exhaust air stream and upstream and downstream of a point of tracer gas injection into the supply air stream. The second component, four tracer gas injection systems, consist of adjustable-speed peristaltic pumps which draw tracer gas from large storage bags and inject tracer through flow meters and into the AHUs. Injection rates are very stable and can be varied over approximately two orders of magnitude. The third major component of the monitoring system consists of 15 small, silent, local samplers which collect samples of air/tracer at a constant rate in one-liter sample bags. The time at which sampling initiates and terminates is programmable. These samplers are used primarily to collect samples at breathing level from various locations (e.g., offices) within the occupied space. Syringe samples of air are also collected manually at each sample location at the end of the sample collection period.

Although a variety of tracer gas procedures can be employed, a tracer gas step-up has been used in all studies conducted to date. In this procedure, a distinct tracer gas is injected at a constant rate into each stream of outside air entering the building or into each associated supply airstream. (With injection into the supply airstream, good mixing between the recirculated air and outside air is necessary for accurate measurements.) Injection and monitoring is continued until tracer concentrations reach steady-state values.

Straightforward calculations based on tracer gas mass balances are employed to determine such parameters as the flow rates of the outside air and supply airstreams and the percent outside air in the supply airstream. Through the application of age distribution theory [7,8], ages of air (i.e., time elapsed since the air entered the building), local ventilation rates (reciprocals of local ages of air), and values of ventilation effectiveness are computed. Through other calculations we can determine the fraction of air at each monitoring point which enters the building through a particular AHU.

To provide an example of the information obtained in these studies, we discuss the results obtained from one of three tests in a complex of three interconnected two-story office buildings (No. 2, 3 and 4) located in Palo Alto, California. In this complex, Buildings 2 and 3 are served by one roof-mounted, variable air volume AHU and Building 4 is served by a similar AHU located within its basement. Air is supplied through ceiling-mounted diffusers and returned through ceiling-level return grills both located in virtually every office. During the monitoring, outdoor temperatures were sufficiently high so that the AHUs were automatically set to maximize recirculation of indoor air, thus bringing a minimum of outside air into the buildings.

The experimental results indicate that approximately 95% of the air within Buildings 2 and 3 enter through the AHU which serves these buildings and that approximately 92% of the air within Building 4 enters through the Building 4 AHU. Thus, there is only a small amount of air flow between the buildings. These results reflect the limited connections between buildings - only one hallway connects adjoining buildings - and indicate that there are no

large flow imbalances which drive air flow between buildings. Based on the data obtained from the local samplers, ages of air and local ventilation rates vary over a moderate range. For example, the ages of air measured with eight local samplers in Buildings 2 and 3 vary between 1.0 and 1.5 h with an average age of 1.3 h. Lesser variability and a somewhat higher age of air is observed in Building 4 where ages of air measured with five local samplers range between 1.5 and 1.8 h with an average value of 1.7 h. The lowest measured local ventilation rate (recipricol of local age of air) of 0.4 h^{-1} is from a hallway which connects buildings. Values for ventilation effectiveness [7,8] can be computed by taking the ratios of age of air in the return duct determined by numerial integration of tracer concentrations as a function of time (1.3 h for Building 2 and 3 and 1.7 h for Building 4 to the average age of air within the building as measured with the local samplers. Ventilation effectiveness values of 1.0 (1.3 ÷ 1.3) and 1.0 (1.7 ÷ 1.7) result from these calculations. Ventilation effectiveness values close to unity, indicate that the air within each zone (Buildings 2 and 3 as one zone and Building 4 as the other zone) is relatively well mixed (e.g., there is not a large amount of short circuiting of air between locations of supply and exhaust).

Other calculations indicate that at the end of the monitoring period, supply air flow rates, outside air flow rates, and percent outside air were approximately 36000 ft^3/min, 10000 ft^3/min, and 28% for Buildings 2 and 3, and 16000 ft^3/min, 3800 ft^3/min, and 24% for Building 4. Finally, the data indicate that there is insignificant leakage of air into these buildings, i.e., virtually all air enters through the AHUs.

PLANNED ACTIVITIES FOR FY 1988

Our largest effort during FY 1988 will be to continue the use of multiple tracer gases to study ventilation within commercial buildings. In a related effort, we will initiate an assessment, based on reviews of available information and modeling, of a technique of ventilation, called displacement ventilation, which is gaining acceptance in Scandinavia. A third effort will be to conduct a follow up study of the effectiveness of radon mitigation systems previously installed in Spokane-area houses. Finally, field studies of selected radon mitigation techniques in central Florida housing will be initiated if funding for this study is received.

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Energy Performance of Buildings*

M.H. Sherman, I. Amarel, P.G. Cleary, R.C. Diamond, D.J. Dickerhoff, D. Dumortier, H.E. Feustel, T. Haugen, H.G. Kula, L.L. Lewicki, M.P. Modera, B.V. Smith, and R.F. Szydlowski

The Energy Performance of Buildings Group (EPB) carries out fundamental research into the ways energy is expended to maintain desirable conditions inside buildings. Our results form the basis of design and construction guidelines for new buildings and retrofit strategies for existing buildings. Our primary areas of research are air infiltration and retrofit research. In this article, the work carried out over the last year is split into five overlapping sections: 1) building energy retrofit research, 2) air infiltration, 3) air leakage, 4) International Energy Agency support, and 5) appliance performance testing. The emphasis in our work is on whole building performance. We collect, model, and analyze detailed data on the energy performance of buildings, including the micro-climate, the building's thermal characteristics, the mechanical systems, and the behavior of the occupants. Because of the multidisciplinary approach we work closely with other groups, both at the Laboratory and elsewhere.

BUILDING ENERGY RETROFIT RESEARCH (BERR)

While new buildings—both residential and commercial—are responding to higher energy prices and stricter energy codes by becoming more energy efficient, the existing stock represents a large area for energy conservation activity. Of the three buildings sectors, single-family, multifamily, and commercial, multifamily has had the least level of activity, and presents some of the greatest challenges. Over one quarter of the U.S. housing stock is in multifamily buildings. The Office of Technology Assessment estimates that while current levels of retrofit activity in multifamily buildings are likely to save 0.3 quads of energy (320 petajoules) by the year 2000, the *potential* savings are more than three times as much. The reasons for this untapped energy savings are complex, and involve institutional as well as technological barriers. While we know something about the performance of retrofits in single-family houses, we have very little understanding of the interactions and performance of retrofits in multifamily buildings. The measured savings from retrofits in multifamily buildings are typically 25-50% less than the predicted savings, with a large spread around the mean.

The Building Energy Retrofit Research project was initiated to address these problems in all three building sectors, single-family, multifamily, and commercial. The Department of Energy has designated LBL as the primary lab for carrying out research in the multifamily sector, although we continue to work in all three sectors. Several of the projects in this area overlap with projects in other areas such as federally-assisted housing, infiltration diagnostics and measurement, and appliance field testing, and are reported in these sections.

Accomplishments During FY 1987

The BERR work can be broken down into four areas: 1) development of a monitoring protocol, 2) development of new diagnostic techniques, 3) analysis of retrofit performance in multifamily buildings, and 4) analysis of behavior of occupants, owners, and managers.

Monitoring Protocol

The need for a standardized set of procedures for monitoring buildings has led to the development of a monitoring protocol for multifamily buildings. An earlier draft of the protocol was used to specify the monitoring procedures used during field tests in multifamily buildings in Chicago, Minneapolis, and St. Paul. The experience gained at these monitoring sites has been incorporated into subsequent drafts of the protocol. The objective of the protocol is to provide a comprehensive standard for data collection and evaluation of retrofit performance. A primary goal for the protocol work is the development of an ASTM and ASHRAE standard for building monitoring. At present the protocol is being reviewed as a draft standard by ASTM. The ASHRAE version is being incorporated into a chapter on monitoring protocols for the *Handbook of Fundamentals.*

New Diagnostic Techniques

While the protocol provides a guideline for long-term monitoring, practitioners and researchers also have a need for short-term diagnostic tests to understand the characteristics of the building shell and mechanical systems. Diagnostics for energy use in multifamily buildings that have been developed or are currently under development include tests of

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boiler efficiencies, distribution losses, shell and inter-apartment leakage (see air leakage section), and appliance efficiencies (see appliance field testing section).

Our diagnostics work in FY 87 included development and analysis of two single-family diagnostic techniques. The first single-family diagnostic was the testing of a technique for measuring air leakage in duct work, specifically, the supply and return side leakage and driving pressures in a central air distribution system (see air leakage section for a more detailed description). The second single-family effort was to test a single-channel wood-stove heat output monitor developed by our group. In collaboration with Pacific Power and Light, we analyzed data taken using this sensor as part of the Hood River Conservation Project (HRCP).[1] The analysis showed that the average efficiency of the wood stove in the field was only 27%, significantly lower than the 50% efficiency that was assumed based on laboratory measurements and estimates based on occupant-reported wood use.

Retrofit Performance in Multifamily Buildings

Our previous year's monitoring work in multifamily buildings in Chicago and St. Paul, Minnesota, has provided a large source of data on the energy characteristics of these buildings. Our work this year has been to develop models that can use this data to evaluate the performance of the retrofits.

Two models are currently under development. The first models the air flow through combustion appliances (i.e., heating and hot water systems) that exhaust through a common chimney, a situation that is typical in multifamily buildings (see Figure 1). The model can be used to predict the performance of retrofits such as vent dampers or flow restrictors based upon the physical configuration and operating characteristics of the system.[2] The second model being developed characterizes the seasonal efficiency of multifamily boilers, taking into consideration the venting issues described above, as well as heat losses through the boiler jacket and to the ground. This model should be capable of providing the data necessary to make recommendations for boiler retrofit or replacement.

As a follow-up to our previous year's collaborative work on monitoring energy use in new Swedish apartment buildings we conducted a study on the appropriate analysis techniques for analyzing the energy consumption data from these buildings.[3]

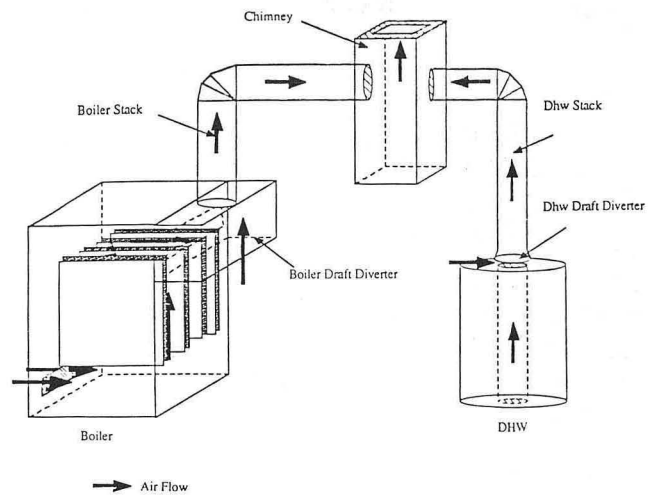

Figure 1. Schematic of air flow paths through two combustion appliances vented through a common chimney. (XBL 8711-4648)

Behavior Studies of Building Occupants, Owners, and Managers

An important aspect of retrofit performance is the related behavioral aspects. Building owners have to make decisions on what retrofits to select, residents modify the retrofits to suit their needs, and building managers take actions that affect the performance of the retrofits. We carried out two projects this year that looked at behavioral effects, the first on the role of apartment managers in determining the energy use in multifamily buildings, and the second, a case study of the energy decision makers in a speculative commercial office building.

The study of apartment managers surveyed several groups and building organizations that have addressed the problems of improving energy efficiency in multifamily buildings through better operations and maintenance. Motivation and feedback were found to be the two key elements in ensuring adequate attention by the building managers. We undertook case studies to examine the basic problems confronting apartment managers, and solutions to some of these problems were documented.[4]

The case study of the two commercial buildings evaluated the role of tenants, managers, and owners in determining energy consumption. Built in the late 70's to showcase new energy technologies, these buildings, known as Enerplex, (see Figure 2) have been intensively monitored and studied to ascertain how they use energy.[5] Our study focused on how

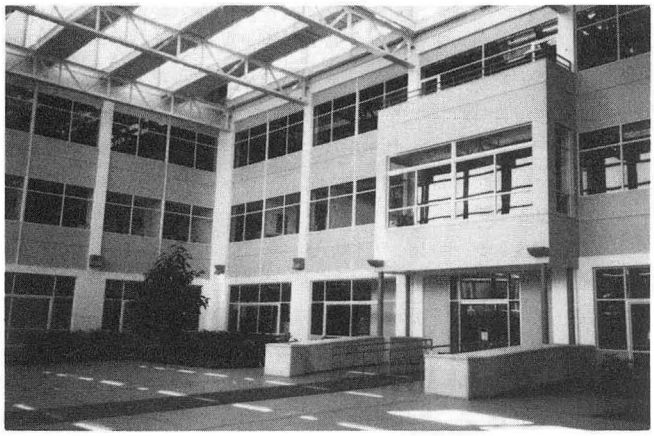

Figure 2. Enerplex office buildings incorporating advanced energy technologies and design strategies. (BBC 8711-9503)

decisions by the owners, tenants, and managers circumvented the intentions of the architects and engineers, resulting in a three-fold increase in actual energy use compared to predicted energy use.[6]

Planned Activities for FY 1988

Our new work will include an investigation of the performance of retrofits in cooling climates. Other plans for the coming year are to continue analyzing the data that has been collected on the monitored buildings, specifically looking at the data on boiler efficiencies. In addition, we will be working with Princeton University in testing new diagnostic techniques as well as preparing a multifamily audit.

AIR INFILTRATION

With improved insulation of the building shell, heat loss from ventilation—whether controlled or by infiltration—has become an even more important fraction of a building's overall heat loss. Infiltration is the flow of outside air driven by wind pressure and thermal buoyancy into the building. Our infiltration is divided into three main areas: 1) infiltration modeling, including the development of a multizone airflow model, 2) multigas tracer measurements, and 3) wind tunnel measurements of the wind pressure distribution on building surfaces.

A number of computer programs have been developed to calculate air flow patterns in buildings. Awareness of the airflow pattern in a building is particularly important when (1) determining indoor air quality for the different zones in a building, (2) evaluating smoke distribution during a fire, and (3) calculating space conditioning loads. Sizing space conditioning equipment is also dependent upon accurate air flow information.

To treat the true complexity of the air flows in a multizone building, extensive information is needed regarding flow characteristics and pressure distributions both inside and outside the building.[7] To reduce the input data required by detailed infiltration models, simplified models have been developed. Most of these, including the one developed at LBL,[8] simulate infiltration associated with single-zone structures.

A high percentage of existing buildings, however, have floor plans that characterize them more accurately as multizone structures. Although multizone models exist, these models need inordinate amounts of input data. Therefore, a simplified multizone model capable of providing the same accuracy as the established single-cell models is being developed at LBL.[9]

Accomplishments During FY 1987

Infiltration Modeling

The first phase of a simplified model for predicting multizone air flows was completed this year. Extensive testing and validation are required however, before the model can be generally used. We plan to validate the model in the coming year through multigas tracer measurements both in the lab and in the field, as well as through a collaborative effort with the *Laboratoire d'Energie Solaire (LESO)* at the Ecole Polytechnique Federale de Lausanne in Switzerland and the EEC Laboratory in Varese, Italy.

In another application, the single-zone infiltration model developed at LBL was used to validate a commonly used rule of thumb that the annual average air change rate is equal to the number of air changes at 50 Pascals divided by 20. Using a set of simplifying assumptions to derive a divisor for this air change rate, typical values ranged from 17 to 23 in various parts of the US (see Figure 3).[10]

Multigas Tracer Measurements

We have designed and assembled a multigas tracer system which is based on a residual gas analyzer using a mass spectrometer (see Figure 4). The system is capable of measuring six different gasses in six independently controlled zones with a complete cycling time of less than five minutes. The system automatically controls the concentration of the tracer gas in each of the zones by using a control

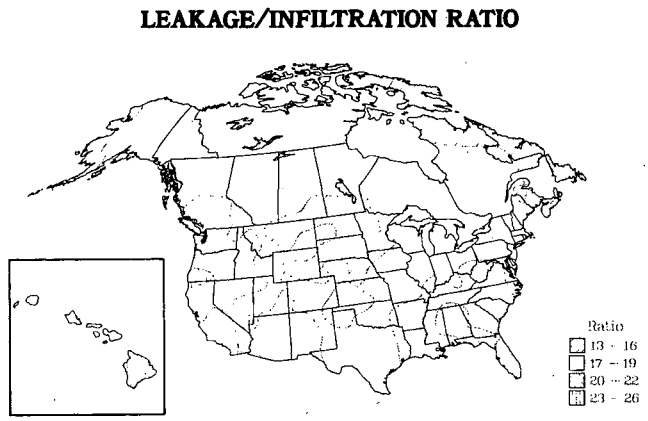

Figure 3. A graph of the United States indicating zones of various leakage/infiltration ratio. (XBL 864-1546)

scheme that keeps the concentrations of the tracer gases stable in the zones.

The multigas tracer system can be used to measure the real-time air flows between different zones in a building, as well as between the different zones and the outside. Although this system could be used as an audit technique, it would probably be too expensive for most field applications. Its primary purpose is to validate mathematical models and diagnostic techniques which, in turn, can be used in more general situations. In addition to using it for validating the multizone infiltration model, we will use the system to validate models of effective ventilation (see below). Other uses include the measurement of air flows in combustion appliances, which was previously not possible using standard spectroscopy techniques.

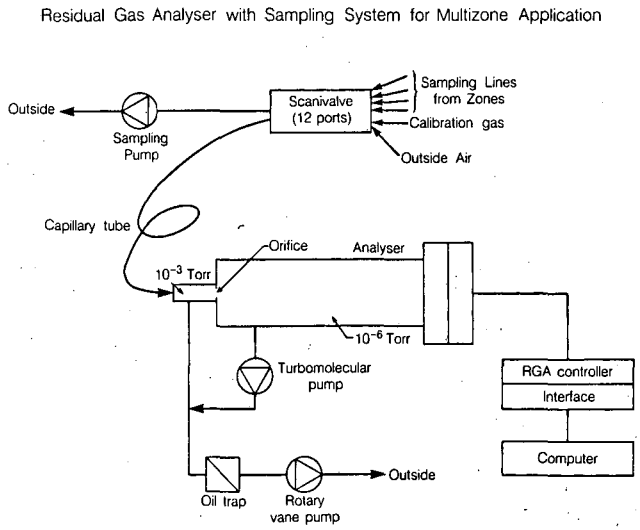

Figure 4. Multitracer gas system for measuring air flows between different zones in a building. (XBL 8711-4647)

Effective Ventilation

The degree to which incoming air mixes with the air in a room depends on the geometry of the space and the ventilation system. This concept has conventionally been called *ventilation efficiency*, and is used in calculating ventilation rates needed for diluting pollutants and ensuring sufficient air quality. In the last year we have expanded the notion to include the fact that time varying ventilation will behave differently from a steady ventilation rate of the same average; we have called this concept *effective ventilation.*

The concept of effective ventilation is especially pertinent to the passive ventilation measurement technique (e.g., perfluorocarbon tracers). This technique is in fact a measurement of the average effective ventilation which can be misinterpreted when the average ventilation is desired.[11] The effective ventilation concept is even more important in multizone environments because of potential mixing problems. The multigas tracer capabilities allow a field measurement of real-time concentration which in turn will provide a verification of the effective ventilation model, and could be used to make a quantitative field test of the perfluorocarbon technique.

Planned Activities for FY 1988

Multizone Modeling

The bulk of the multizone infiltration modeling work will be done in two parts: 1) cooperative validation work at the EEC Laboratory in Varese; and 2) preparation for the COMIS workshop in FY89. COMIS (Conjunction of Multizone Infiltration Specialists) is a year-long international workshop scheduled to take place at LBL during FY89. Experts from approximately 10 different countries will work together to complete the problem of predictive modeling of air flow in multizone buildings. The intended outcome is a general purpose computer code for use by designers, policy makers, researchers, and others.

Multigas Tracer Measurements

In the coming year we plan to start using the Multigas Tracer Measurement System (MTMS) in the field. These measurements will be done in single-family and multifamily buildings and will allow verification of the effective ventilation concept and provide input data for the multizone infiltration models.

Effective Ventilation

The effective ventilation work will expand to include multizone environments as well as to examine the transport of specific pollutants, such as radon. The comparison of effective ventilation predictions to the measurements using the multigas tracer measurement system will begin after completion of the field measurements.

AIR LEAKAGE

The process of air flowing through unintentional openings is called air leakage. In buildings, air leakage occurs through openings in the building envelope, in mechanical systems, and in between building zones. Air leakage flowrates depend both on the air tightness of the building component as well as on the pressures driving the flow. The fan pressurization technique, i.e., blower-door testing, has evolved over the past ten years as the standard technique for characterizing the air tightness of building envelopes. We have started developing techniques to measure the air tightness of mechanical systems (such as air ducts) as well as the air tightness of internal partitions between zones (such as in multifamily buildings). For all three types of air leakage, the measurement and study of air tightness allows us to characterize buildings, better understand ventilation and space conditioning, evaluate the performance of mechanical systems, and estimate the effectiveness of air-tightness retrofits.

Our air leakage research can be divided into three areas: leakage characterization, measurement techniques, and consensus standards. Our leakage characterization effort involves collecting and analyzing measured leakage data, as well as understanding the fluid dynamics of air leakage. As part of our measurement technique research we have developed an alternative technique for measuring building envelope airtightness, AC Pressurization, and are presently developing techniques for measuring the air leakage in residential duct systems and multizone buildings. Finally, we are transferring our experience by participating with professional societies in the formation of consensus standards.

Accomplishments During FY 1987

Air leakage research efforts in FY 87 focused on the development of measurement techniques covering three types of leakage: envelope, duct-system, and multizone. The envelope leakage research has concentrated on quantifying the effects of wind on both fan pressurization and AC pressurization measurements. Wind-induced pressure variations add uncertainty to the measurement, which we measure using a portable test building, the Mobile Infiltration Test Unit (MITU). Our experiments with MITU have shown that the effects of wind on fan pressurization measurements can be significantly attenuated by using a four-wall pressure averaging probe developed in Canada. The MITU tests also indicated that the leakage area measured by AC pressurization did not vary with the wind, up to wind speeds of 8 m/s (18 mph). As this result is encouraging, an analytical examination of the effects of wind on AC pressurization is planned.

A theoretical and experimental investigation of a new envelope leakage measurement technique was initiated in FY 88. This technique, known as pulse pressurization, determines the leakage characteristics of the envelope from the decay of the building pressure from an elevated value down to its steady-state value. Preliminary experiments performed in MITU showed that the the technique has the potential for wider application, although further demonstration of the theory and development of a practical prototype remain to be performed.[12]

As part of a larger multifamily retrofit research project, initial experiments were performed with three potential multizone leakage measurement techniques. Rather than testing an actual apartment building, as was done in FY 86, the experiments were performed under controlled conditions in a single-family house that had been divided into two zones with a panel having known leakage characteristics. Two of the techniques tested used blower doors, whereas the third technique was based upon the AC pressurization apparatus. The two blower techniques differed in the way the pressure differences between the two zones were varied, and the manner in which the data was analyzed. The results of these tests will be analyzed, and recommendations developed in FY 88.

One of the major accomplishments of FY 87 was the measurement of supply and return side leakage in a central air distribution system and the characterization of the pressures driving the leakage in that system. Determining the split of duct-system leakage between the return and supply sides of the fan is important both because the energy penalties associated with this leakage can vary by a factor of four depending upon the leakage split, and because the indoor air quality implications depend upon this split.

During FY 87 we also made use of the air tightness database that was compiled during the past several years.[13] This database, which contains 1100 measurements on 750 houses in 110 different zip codes, was used to estimate the total leakage area of

duct systems, which was found to average 190 cm^2 for 90 California houses.

As part of our work with professional committees and organizations, we were involved with two standards-writing organizations: the American Society for Testing and Materials (ASTM) and the American Society of Heating Refrigeration and Air-conditioning Engineers (ASHRAE). We participated in several activities in ASTM during FY 87, including the modification of Standard Test Method E-779, "Determining Air Leakage Rate by Fan Pressurization" to include effective leakage area as part of the standard. Standard E-779, after public review, was published as an official ASTM standard in FY 87. We are now participating in four new standards in ASTM. We are continuing to work with ASHRAE standard project 119P, which is intended to promote energy conservation by setting maximum values for air leakage in detached single-family residential buildings.

Planned Activities for FY 1988

Air leakage research efforts in FY 88 will focus on analysis, interpretation, and documentation of the experiments performed in FY 87. These efforts include analysis and further testing of the multizone, duct, and pulse-pressurization measurement techniques.

The other focus of air leakage research in FY 88 will be in leakage characterization. The objective of this work is to develop a workable physical model for air flow through large apertures submitted to dynamic pressure conditions. This more basic work has application both to our two dynamic leakage measurement techniques, AC pressurization and pulse pressurization, as well as to the dynamic flows associated with natural ventilation. In addition to our experimental examination of flow profiles this work will also include theoretical modeling efforts in collaboration with the Royal Institute of Technology in Sweden.

The standards work will also continue during FY 88. In particular, during FY 87 ASHRAE standard 119 was put out for public review, and is expected to be published in FY 88.

IEA SUPPORT

In response to the 1973-74 oil crisis, the OECD countries formed the International Energy Agency. As part of the implementation agreement, technical annexes were created to enable countries to work together on problems of mutual interest. To date, thirteen technical annexes have been formed. Our group has been representing the U.S. on Annex V, the Air Infiltration Centre.

Accomplishments During FY 1987

The U.S. has been one of the most active members of the Air Infiltration and Ventilation Centre (AIVC). As the U.S. representative, we provide interested parties with information material, e.g., the quarterly published Air Infiltration Review, which is sent to over 640 U.S. researchers and professionals. We also distribute the AIVC Technical Notes to interested parties.

During FY 87 the Air Infiltration and Ventilation Centre responded to approximately 120 inquiries from the U.S. and delivered over 600 copies of technical papers held in their library of some 2,200 ventilation-related papers.

Planned Activities for FY 1988

There are two new annexes being considered by the Executive Committee; one on moisture and the other on the fundamentals of air flow patterns. LBL is qualified to participate in either.

APPLIANCE PERFORMANCE TESTING

Gas and electric utilities use a large array of information for forecasting future energy demands. This project is concerned with the projection of energy demand due to major appliance operation in single-family residences. These are gas and electric domestic hot water heaters, refrigerators, central air conditioners, and central gas furnaces. Although some data is available for residential end-use energy consumption there is no data base available on major appliance field performance. Future energy demand is dependent on knowledge of actual appliance efficiencies changes due to factors such as long-term degradation.

Accomplishments During FY 1987

We have conducted a project in conjunction with Pacific Gas and Electric, the California Energy Commission, and DOE to develop and test procedures that are applicable for field appliance performance testing. A major goal of the study was to compare the measured and the rated efficiencies of the target appliances.[14] Another goal of the study was the development of simple techniques for a large-scale survey of appliance efficiencies.

Methods development, conducted in early 1986, investigated several techniques for duplicating laboratory appliance efficiency indicator measure-

ments in the field. A total of 61 single-family residences located in north-central California were monitored during the summer of 1986 and winter of 1987.

Refrigerators

For refrigerators the only efficiency indicator is the monthly energy consumption, based on a week-long measurement of energy consumption and freezer compartment and ambient temperatures. Figure 5 compares normalized specific energy consumption with unit age and with the applicable California standards, where specific consumption is the measured electricity consumption adjusted for volume, allowing all volumes of refrigerators to be compared in the same figure. Newer units clearly consume less energy than the older units.

Domestic Hot Water Heaters

A large amount of scatter is evident in Figure 6, which compares measured recovery efficiency with unit age and with the applicable California standards. There is no clear trend of efficiency with age. Some 30-year old units are as efficient as 1-year old units. Some of the low values are attributable to thermosiphon loops or other loss mechanisms which would not be found in a laboratory test setup, although they may be common in the field.

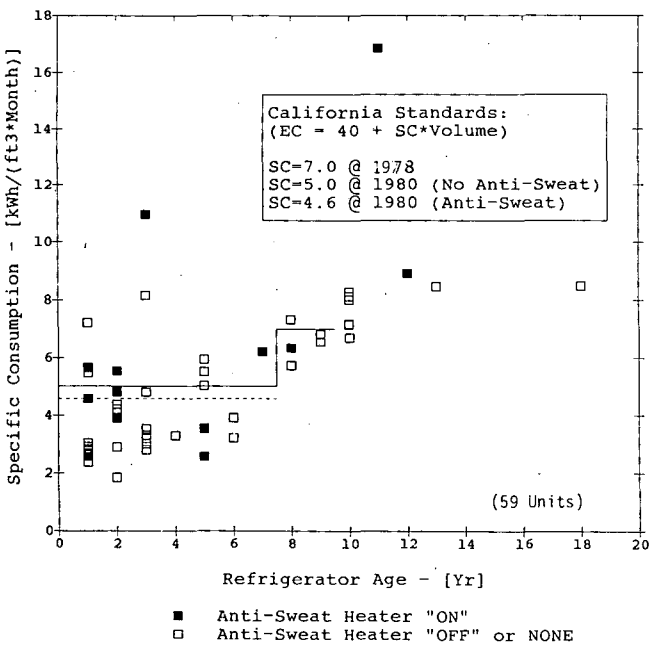

Figure 5. Refrigerator electricity consumption by age of refrigerator. (XBL 8711-4646)

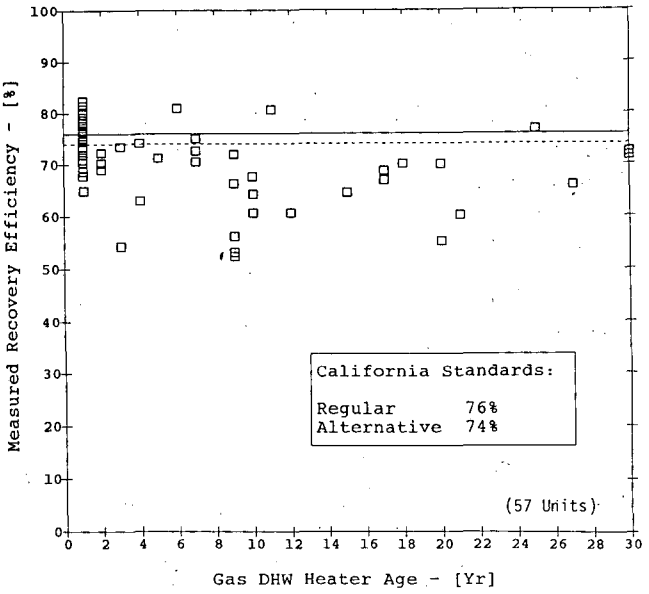

Figure 6. Measured recovery efficiency of gas water heaters by age of appliance. (XBL 8711-4645)

Central Air Conditioners

This study attempted to determine the Energy Efficient Ratio (EER) and Seasonal Energy Efficient Ratio (SEER) indirectly by measuring the heat rejection at the outside condenser coil. This technique was chosen due to the difficulties associated with field measurement of latent heat removal. The outside coil is more accessible for sensor installation and does not have latent heat loads. Three different methods of measuring condenser unit air flow rate were used. The high turbulence and pressure sensitivity of the the fans resulted in condenser-coil air flow measurement uncertainties on the order of 25%. Given this level of uncertainty in the data, it is clear that the experimental methods require considerable improvement.

Central Gas Furnaces

Figure 7 shows the variation of measured furnace efficiency with unit age, and its relationship with the applicable California standards. The older unit steady-state efficiencies cluster around 75%, while newer units seasonal efficiency is generally better than the requirement.

Planned Activities for FY 1988

The project was completed in FY 1987, and the only additional work will be the publication of the results.

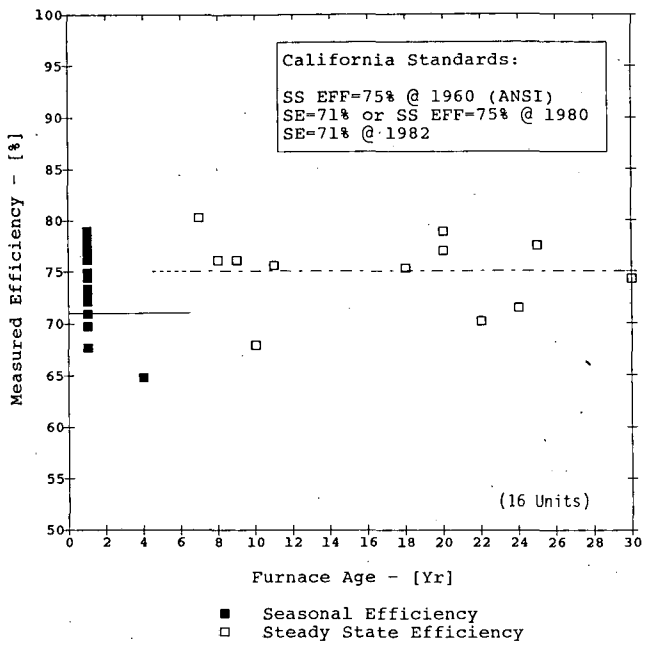

Figure 7. Measured efficiency of gas furnaces by age of appliance. (XBL 8711-4644)

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Indoor Radon

LBL-17598 Rev.
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