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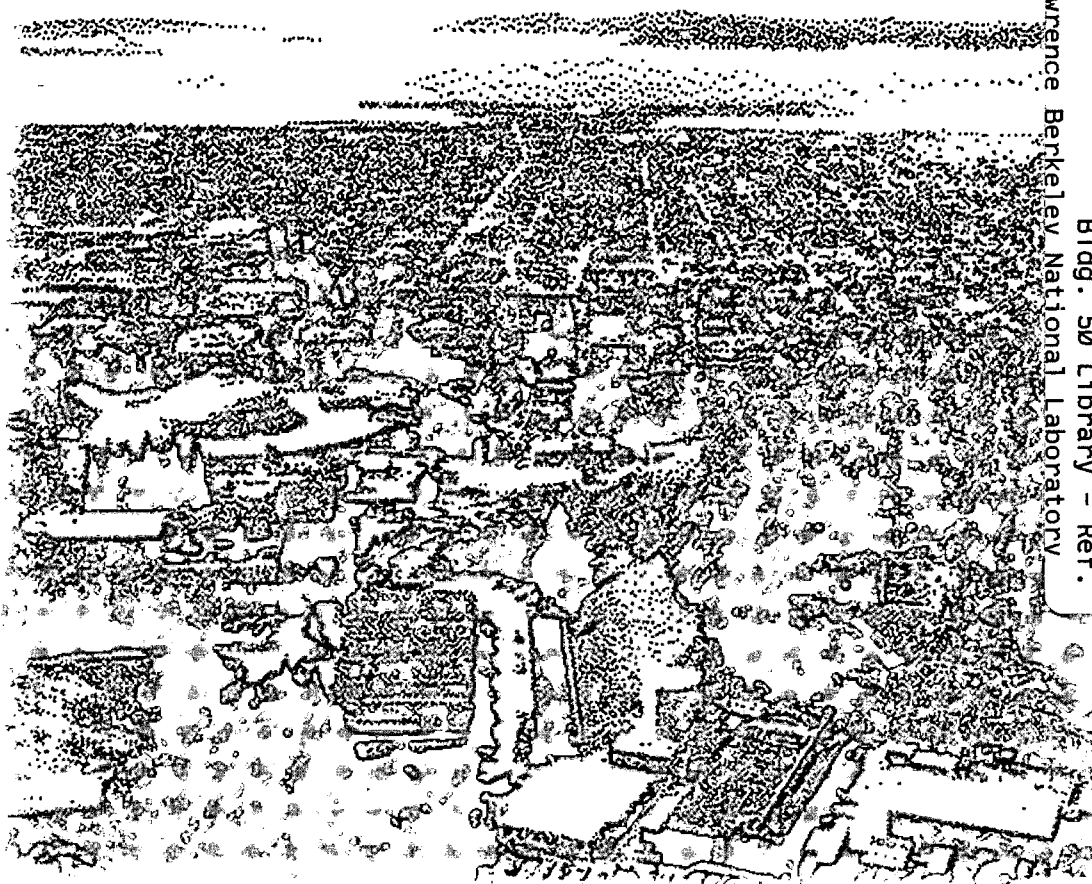Olsen, T H
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**Environmental Energy
Technologies Division**

March 1999

DISCLAIMER

Toward a Virtual Building Laboratory

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INTRODUCTION

Buildings account for about one-third of all energy used in the US and about two-thirds of all electricity, with associated environmental impacts.(EIA 1996) After more than 20 years of DOE-supported research universities and national laboratories, a great deal is known about the energy performance of buildings and especially their components and subsystems. The development and market introduction of improved energy efficient technology, such as low-E windows and electronic ballasts, have helped reduce energy use, and the resultant savings will increase, as use of the new technologies becomes more widespread. A variety of approaches to speed market penetration have been and are being pursued, including information dissemination, research to evaluate performance and development of computer tools for making energy performance simulations available to architects and engineers at the earliest design stages. Public-domain computer building energy simulation models,(BLAST_Support_Office 1992; Winkelmann, Birdsall et al. 1993) a controversial idea 20 years ago, have been extremely successful in facilitating the design of more energy-efficient buildings and providing the technical basis for improved state building codes, federal guidelines, and voluntary standards. But the full potential of savings, estimated at 50% of current consumption or $100 billion/year, (Bevington and Rosenfeld 1990; Todesco 1996; Holdren 1997; Kolderup and Syphers 1997; ORNL, LBNL et al. 1997) will require that architects and engineers take an integrated look at buildings beginning in the early design phase, with increasing use of sophisticated, complex and interrelated building systems. This puts a greater burden on the designer and engineer to make accurate engineering decisions.

The cost and risk of failure in the design of buildings is large. While $100 billion/year for wasteful energy use is a large social cost, other, more individualized, costs loom larger in the eyes of practitioners. Sick building syndrome (SBS), estimated to cost an additional $50 billion/year, (Fisk and Rosenfeld 1997) can occur throughout a building's life, undermining worker productivity and increasing health care costs. While building tenants usually bear these costs, when SBS occurs immediately upon occupancy in a new building it can become a liability for the designer or builder. This acts as a powerful economic incentive for designers and engineers to stick with known methods that have avoided this poorly understood problem in the past. There is an additional large penalty in specific buildings where serious design flaws necessitate costly retrofit shortly after construction. In the face of these risks, architects and engineers are reluctant to try new approaches, even when these promise savings, better buildings and the social benefits of reduced energy use, because of the liability associated with unforeseen negative effects on occupants. To reduce these risks requires the ability to determine local health and comfort effects on building occupants, including those that result from unforeseen consequences of the building design. This is beyond the capacity of current building simulation models.

One conceptual approach is to build full-scale prototypes of each new design. By building, testing and then refining each prototype design, it should be possible to develop solutions that provide the desired energy performance and reduce health problems. However, the cost of such full-scale prototyping is prohibitive. A variant of this approach, construction of a laboratory to study whole-building effects, was also found to be very expensive.(Drost, Crawley et al. 1988).

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An alternative approach is to improve building simulation modeling techniques to the point where they could predict local health and comfort effects reliably. Two developments give reason to expect that progress is possible in this area. The first has been in the area of lighting design. In the design of lighting and daylighting systems it is well known that the response of the occupant—both in terms of visual comfort/performance and aesthetic/architectural appeal—is of paramount importance, and an important component of research aimed at energy-efficient lighting has been directed at developing methods of simulating lighting in a computer rendering. This has resulted in the program *Radiance*(Ward 1994), which can produce computer renderings of lighting in complex architectural spaces that are nearly indistinguishable from photographs. The clear implication of this work is that in the foreseeable future it will be possible to model visual environments by computer with near-complete physical realism. The second development has been the great advance in the techniques of computational fluid dynamics (CFD) in the interval since the design of the current generation of building simulation models. Processes that then could not be modeled are now tractable, and CFD techniques developed primarily in aerospace applications are just beginning to be applied to building problems (Baker, Williams et al. 1994; Kato, Murakami et al. 1995; Negrão 1995; Chen 1997).

This report describes the beginnings of an exploration to determine how CFD developments can be utilized to bring building simulation modeling capabilities to the point of realistic physical simulation necessary to predict building design success. The general idea is to bring the numerical simulation of a building to the level of realism and reliability that would allow one to do numerical experiments and prototyping as a substitute for full-scale testing—a Virtual Building Laboratory—in the same way that numerical simulations have sometimes replaced wind tunnel testing in the aerospace industry.

CONCEPTUAL MODEL

The project began by constructing a picture of what the final resulting virtual building model might look like, and how it relates to the current state of the art building simulation model (BSM). It is expected that something resembling this picture might emerge only after extended effort by multiple institutions in collaboration; nevertheless, formulating the picture is useful for defining goals and initial strategy.

Limitations of Current Models

Current building simulation models (BSM's) are essentially models of transient heat conduction in the building's physical shell, driven by (a) solar radiation, (b) outdoor temperature and other climatic variables (such as wind speed and direction and humidity), (c) effects of auxiliary energy dissipating equipment in the building (such as lights, appliances, office equipment, etc.) and (d) the action of the building climate-control equipment. The latter two categories include the effects of comfort objectives for the building interior (i.e., controls), scheduling, etc. Because a building's physical shell has a long conductive time constant—typically in the range of hours to days—the time step of existing building simulation models is large, typically one hour.

In these models the internal air is treated as a highly conductive, low density solid with insulated surfaces (well-mixed air core with "film coefficients"). While this is a reasonable approximation within the current BSM objectives, it is well known that it produces unrealistic surface temperatures, (Bauman, Gadgil et al. 1983) and since therefore BSM's can predict neither local radiative nor air temperatures, prediction of local thermal comfort is not possible.

Two examples will show how the buildings modeled in current BSM's fall short of the reality. The first is the actual operation of a single-family residence with forced-air heating in winter. At

some point, the air temperature at the control thermostat (assuming the house is a single zone) reaches the lower control set point, and the heating system is switched on. The air is circulated and heated by the heating system, and after some number of minutes the air temperature at the thermostat reaches the upper control point, and the heating system switches off. At that point, the air in each room is well-mixed (assuming good air distribution) and has considerable turbulence, although on the average the fluid is at rest. In the room containing the control thermostat the air temperature is at the upper control point, and in other rooms the air temperatures will depend on the balance of the air distribution system. Assume for simplicity that they are all at the same temperature. The air is now warmer than the solid surfaces in the room, so natural convective flows will be set up; in addition, the initial turbulence will be dissipated. The air temperature distribution in a room will be determined by the competition between natural convection, which tends to produce vertical stratification, and the remaining initial turbulence, which promotes mixing. These processes dominate the heat loss to the envelope (which causes warming of the surfaces and consequent changes in radiant exchange between them) until the cooling air at the thermostat again reaches the lower control point, reinitiating the cycle. The length of the cycle might be on the order of ten to twenty minutes, and depends on the outdoor temperature and the level of insulation of the house. Solar radiation complicates this picture, but does not change it essentially.

One sees, then, that the air in a real residence is in a constant state of thermal oscillation that is rapid compared to the thermal response time of the building shell. The long-term building heat loss is an average over this oscillation, and a BSM calculates this average by assuming a time-averaged condition for the air. But the degree of error contained in this assumption and the question of other consequences of this oscillation (e.g., thermal comfort) are questions that cannot be answered with a current BSM.

A second example is that of a large atrium in a commercial building. Given its uniform air temperature assumption, a BSM can calculate the energy flows necessary to condition the entire atrium space, but generally it is not desirable to do this, both from an economic and an energy-efficiency standpoint. Instead, only the small, occupied portion of the atrium (e.g., at the bottom and possibly on the sides) is conditioned. The equipment loads necessary to do this are not calculable from a BSM, and cruder methods must be used. Given the downside risk in design and the HVAC industry's historic use of safety factors, one suspects that these systems are considerably oversized, with consequently higher first costs and lower efficiency than would be possible with accurate calculation.

A Complete Physical Building Model

Constructing a complete physical building model must begin with a reexamination of exterior as well as interior conditions. Although the thermal time constant of the building shell is long, small-scale variations in conditions both in space and in time may have an effect. The detailed flow fields over the building exterior affect surface heat transfer coefficients, while the detailed pressure field affects air leakage as well as ventilation intakes and exhausts. Both of these fields depend on the local environments provided by topography, neighboring buildings, and vegetation, as well as atmospheric conditions at some distance from the building. Nearby sources of moisture or pollutants—including the building's own exhausts—combined with the flow fields could be important for determining ventilation effectiveness. From the standpoint of building design, it is important to simulate a realistic range and probability spectrum of conditions on the building exterior rather than the actual conditions.

These considerations suggest the possibility of using a large-scale CFD calculation to determine the building exterior flow, pressure and concentration (i.e., of moisture or pollutants) fields, taking account of the building shape, surrounds, and the limited and relatively simple ways (e.g., cooling tower or exhaust plumes) in which the building affects its surroundings.

A detailed simulation of ambient radiation incident on the building is also necessary. Since this is already an issue of recognized importance in BSM's, it does not need elaboration here.

The physical structure of the building remains a long-thermal-time-constant (primarily) transient heat conduction system that should (at least in some cases) be modeled in 3D. It provides a very important simplification to the overall problem: it acts as a low-pass filter to prevent all but the slowest-varying fluctuations in the external conditions from influencing the building interior (with some exceptions to be noted below). Likewise, variations in interior conditions (such as heating, cooling or ventilation demand and heat dissipation) can have effects on the exterior conditions only in ways that are very local (e.g., window, door, vent intake or exhaust openings), or slowly-varying (e.g., building skin temperature on a winter day with low wind). There are cases where the building itself is expected to be a significant driver for its exterior conditions. A high-rise, sunlit building in the summer in Arizona has been shown to produce significant natural convective exterior boundary flows under low-wind conditions, (Yellott, P. V. R. Schuyler et al. 1979) but here the dominant influence was incident solar radiation, not interior conditions.

These considerations imply that the causal scheme generally postulated in BSM's will still be valid even if one assumes a very much more detailed level of physical modeling. The climatic conditions of wind, solar radiation, etc. far from the building environment provide the driving conditions that, together with the geometry of the building and its surrounds, determine the local conditions at the exterior building surfaces. This means that (with the possible exception of limited special cases) the local exterior conditions can be produced by a time-marching solution of the driving equations, an important simplification. These local exterior conditions are the drivers for the building physical structure; this in turn produces slowly-varying quantities, the indoor surface temperatures, which are among the drivers determining the building interior air flow and heat transfer.

The state of the interior air is determined by the following: (a) the interior surface temperatures, (b) air flows into and out of the interior driven by building climate-control equipment, (c) air flows to or from the exterior through windows, doors, vents and leaks, (d) energy dissipation within the interior air (e.g., by lights, appliances, people, etc.) and (e) production or accumulation of gasses (including water vapor) within the building exterior. The latter is intended to include all processes that modify the concentrations of gasses other than the constituents of dry air within the building, excepting those included in (b) and (c): the production of pollutant gasses by chemical processes, outgassing of materials, humidification/dehumidification within the interior air volume, etc. If it is possible, desirable or necessary to divide the interior air volume of the building into separate zones (as will frequently be the case) then to the above one must add interzone transport. It is important to note that the interior surface temperatures above are not independent variables: they depend both on the state of the physical structure (which includes interior radiation exchanges) and on the state of the interior air, a point to which we will return. We also note that (c) above represents the exception allowing short-time-scale variations in exterior conditions to influence the building interior air; while we will neglect the reverse effect, it may sometimes be of interest (e.g., in studying building exhausts, catastrophic release of pollutants, etc.).

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This discussion is summarized in Figure 1, which indicates the breakdown of a complete building physical model into submodels and the interrelations between them. A possible procedural structure for such a model is shown in Figure 2.
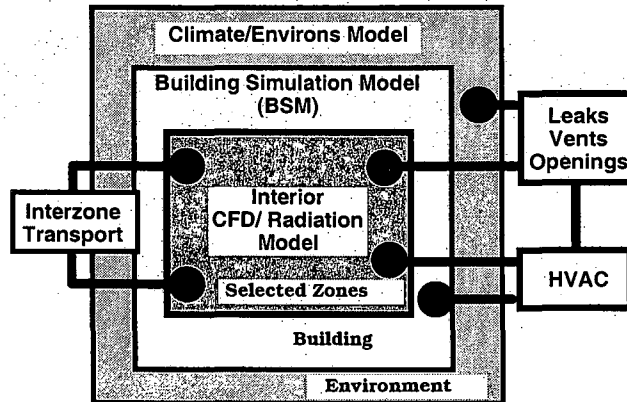

Figure 1. Modular Structure of a Complete Building Physical Model. Flow of information across the Environs/BSM boundary is primarily unidirectional, while model interdependence across the BSM/Interior CFD boundary is bidirectional.
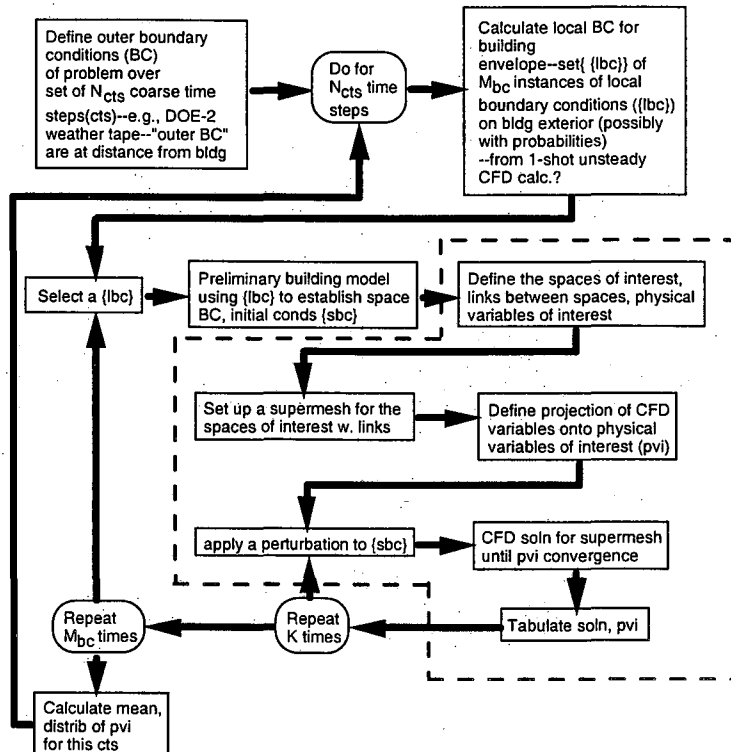

Figure 2. Conceptual Implementation of a Complete Physical Building Model Calculation

First Steps: Defining A Building Interior Model

Among the components of a complete building physical model, a realistic interior model of the building interior environment, as indicated by the dashed-outlined area in Figure 2, stands out as the most fruitful place to begin. There are two reasons for this; on one hand, this is the area where least work has been done, and on the other, this is the area where improved capability will most directly affect the ability to predict the phenomena of greatest interest: comfort and health effects on occupants. By contrast, as long as the isothermal-internal-air assumption is not changed, modeling the building physical shell is a well-developed subject under continuous extension; some existing models even include 3D capabilities. And there is a vast literature on forced CFD calculations in exterior environments originating in the applications to aerospace design, weather prediction, and wind loading of structures. Once a realistic interior model is in hand, then, it should be possible to proceed outwards and find already well-developed components to be adapted to the modeling effort.

There are two separable aspects to the interior environment, visual and thermophysical. It is well known that a realistic representation of the visual environment is vital to the design and evaluation of lighting and daylighting systems, and these have a large impact on building design. There is already an active program of research and development of the program *Radiance* (Ward) to deal with this need. While the Virtual Building Laboratory includes philosophically the further development of realistic simulation of the visual interior environment, while some of the techniques for calculating the accurate spatial distribution of radiation within a building may be applicable, and while the *Radiance* spatial rendering provides interesting possibilities for the display of thermophysical information, there is no physical reason that a full visual simulation needs to be included in the building interior model. Some of the consequences of the visual simulation will certainly need to be incorporated into the physical simulation. But in general we will concentrate here on the thermophysical simulation, assuming a separate visual simulation.

It is clear that a realistic building interior model must replace the well-mixed-air assumption of BSM's with a CFD calculation in 3 dimensions. This solution must incorporate the correct boundary conditions, that is, a physically correct representation of the interaction between the physical building structure (including its HVAC system and leaks, vents and openings) and the interior air. In addition, the model should be designed with the idea that it will be first a tool for building research and eventually become a tool for design. This means that it should be designed to accommodate those geometrical complexities that occur in buildings, should provide easy set-up and modification of problems, and should not be too labor-intensive to use. Finally, the model should have a property we metaphorically term imperialism: as will be shown, complete CFD for the full interior of a very large building is beyond even present supercomputer capacity. The model should conquer as much of the problem as possible given present resources, and should be capable of extending its domain further given increased future resources.

Boundary Conditions

The air in a building interacts with its surroundings in either of two ways: (1) by flow through openings (either inlet/outlet vents of the HVAC system or through openings communicating ultimately with the building exterior—windows, doors, leaks, etc.) and (2) by heat transfer at surfaces. In general, we should include as part of the "surroundings" equipment, furniture, occupants, etc., contained within the air volume, but this does not introduce any new kinds of boundary conditions. For conditions of type (1) either the velocity or pressure distribution over the opening, together with the temperature and concentration distribution for inward-flowing air, provides the boundary condition. For conditions of type (2) there is of course the requirement

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that air velocities at the surface are zero, but the temperature and its normal derivative at the surface are determined by the equilibrium between (a) heat flow between the surface and the air, (b) solar radiation arriving at the surface and absorbed there (having entered the building through a window or opening, and possibly having undergone one or more reflections), (c) long-wave infrared radiation exchanged with other surfaces, and (d) heat conduction into or out of the surface. The boundary condition is complicated by the fact that (a) depends on the surface convection coefficient, which is determined from the solution of the CFD problem. Moreover, (d) depends on the physical building model, or at least the nearby portions of it (heat capacity and temperature distribution in the adjacent envelope elements).

A particular aspect of buildings is that, while loads on a space (i.e., heat loss in winter, heat gain in summer) occur primarily through conditions of type (2), control of the indoor conditions may be accomplished through either type of boundary condition. Conditions of type (1) (forced-air conditioning systems) are usual; when control is exercised through conditions of type (2) it is generally *for very localized areas* (e.g., heaters, radiators). This points up yet another link between the building interior and its physical structure (modeled by the BSM). The controlled boundary conditions (flow rates, inlet temperatures and concentrations for forced air, surface temperature as a function of time for heaters, etc.) will be set by one or more chosen measures of the interior conditions (e.g., air or comfort temperature at a thermostat, occupant sensors controlling heaters or lights, CO_2 sensors controlling ventilation, etc.) in conjunction with the building control system and equipment inventory (all modeled by the BSM).

Usability

A CFD-based building interior model that is ultimately to be usable in building design must be adapted to the way buildings are designed and built. This is quite different from the area of highly engineered products to which CFD is normally applied. Many architectural spaces are simple, and most buildings are highly modular and repetitious assemblages of relatively simple components. Yet the assemblage quickly gives even a small building a high degree of geometric complexity. This makes constructing an abstract geometric representation of a building a very arduous task. Changing the design can be equally arduous, yet the whole goal of the modeling effort is to discover improved designs; introducing new obstacles to making changes would be counterproductive.

Constructing a CFD building interior model will be a difficult and highly technical task. Once a physically satisfactory calculation has been achieved, a large body of computer code will have been assembled, and making major changes will be difficult and expensive. Thus, although for research purposes a great deal of inconvenience in model construction could be tolerated, the eventual goal of wide usability means that one must keep sight of ease of model specification and alteration at the outset and throughout.

Similar considerations apply to the process of applying the calculation to the design. Using CFD calculations currently requires expert knowledge for setting up problems and obtaining solutions, and is a time-intensive task for those experts. It will be necessary to simplify this process to the point where routine use in the building design and engineering process becomes practical. This is in itself a formidable research task.

Model Imperialism

The approach that we term model imperialism is not a new one, especially in the field of CFD. For example, weather prediction programs, which include large-scale CFD calculations, are continually increasing the time span and accuracy of their predictions as computer resources

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increase and understanding of the meteorology improves. Similarly, rather than aiming at a model for a particular type of architectural space (e.g., an atrium), we seek to model as much of a building interior as possible, and to extend the solution domain as capabilities improve. The most immediate consequence of this approach is that the efficiency of the numeric solution method becomes a high priority.

CONSTRUCTING THE BUILDING INTERIOR MODEL

Having outlined the final building interior model, we now address the starting point on the research path that will lead to this goal.

The Research Challenge

While the development of CFD techniques makes it possible to begin a building interior model, the precise set of equations to be solved is not yet a settled issue. While the equations of fluid dynamics, which are essentially the consequences of energy and momentum conservation, are perfectly general and well known, it is not possible to solve these equations for the conditions of interest without introducing an empirical model of turbulence. The most widely used turbulence model is the k-ε model(Launder and Spalding 1974), which works best when turbulence is strong. The flow in building interior spaces is almost always turbulent to some degree, both because of the large spatial dimensions and because inlets of conditioned air usually produce turbulent jets. In addition, heat-dissipating appliances and occupants produce thermal plumes, and occupant motion creates turbulent wakes. However, the turbulence is not strong everywhere, and consequently the k-ε model does not necessarily predict the correct flow.(Nielsen 1998; Xu and Chen 1998).

Buildings span a huge range of sizes. The average US residence has a volume on the order of 700 m^3; the average commercial building, 5000 m^3. But the largest commercial building is over 3 X 10^5 m^3. A 3D CFD calculation will require on the order of one point per 0.1 m, or 1000 points per m^3. In some regions a smaller density may be possible, but, on the other hand, millimeter or better resolution along the perpendicular dimension is necessary near surfaces if one wishes to determine the heat transfer coefficient. A large CFD calculation on a supercomputer is typically on the order of a half-million points; for example, a reported calculation using 3.5 X 10^5 points required 50 hours on an 8 GFLOP supercomputer(Kato, Murakami et al. 1995). This means that modeling a complete average residence is currently feasible, but an average commercial building (much less a large one) is not. On the other hand, a future thousand-fold increase in computer speed is by no means impossible.

Solving the thermal radiative exchange among the interior surfaces is a calculation that can be of a difficulty comparable to the CFD solution. If the network of points filling the volume has N points, the boundary points on the surfaces will be of order N$^{2/3}$. In the worst case (e.g., a single large atrium) most of these points will be able to exchange radiation, resulting in a number of interacting pairs on the order of N$^{4/3}$; i.e., there will be a radiative exchange matrix that is N$^{2/3}$ X N$^{2/3}$. In order to solve the radiative exchange it is necessary to invert this matrix, which is not in general sparse. Since as is well known it takes on the order of M^3 operations to invert an M X M matrix, this will take on the order of N^2 operations. Fortunately, this inversion only needs to be done once, since the view factors do not depend on temperature. However, each iteration of the boundary temperatures will involve a matrix multiplication, which is N$^{4/3}$ operations. Since for an efficient solution method the CFD solution time is expected to grow linearly with N, (Brandt

1981) the radiation calculation will eventually be a comparable computational load, or even dominate.

However, the actual dependence of computational effort on building size may be more complex than this argument suggests. The above type of scaling argument applies to spaces rather than buildings. A building will in fact be a linked set of spaces, each of which contains N_i net points. But in addition to the normal linkages between the spaces through conduction, convection and radiation, there will be linkages caused by conduction through the building shell and the action of HVAC equipment and controls. Each of these has its own time scale, which may be quite different from the radiative and CFD time scales. The building conduction time scale will generally be long, and this may be a simplification in the propagation of the solution in time, allowing a quasi-static approximation. However, finding an initial self-consistent solution from which to begin the propagation will require dealing with the extra stiffness due to this very different time scale. In general, one can say only that CFD/radiation problems in a building have a quite unique structure, and solution techniques that are designed to adapt to this structure are likely to be much more efficient and successful than those that are not.

The preponderance of work on numerical solution of CFD problems has been for high-speed, forced convection. Examples are aerospace design and engineering for wind loading of structures. These solutions only require the solution of the three equations of fluid dynamics deriving from momentum conservation (the Navier-Stokes equations) together with the continuity equation and the equation of state for the fluid. Another significant fraction of work has been on combustion, which does require the inclusion of temperature and buoyancy forces, necessitating solution of the full set of fluid dynamics equations (i.e., including the equation deriving from energy conservation). In both of these areas the equations for the velocity field have a hyperbolic character; that is, one can specify initial velocities on some surface and march them through the problem to determine the consequent flow field.

Modeling the air flow inside a closed volume such as a building space introduces the possibility of recirculation, which means that the flow at a given point must be self-consistent: fluid arriving at that point has originated at the same point at a previous time. To put it more technically, problems involving closed spaces and buoyancy-driven flow require solution of a system of equations that is partially elliptic or parabolic. Solving such a system numerically requires more computational effort than solution of a hyperbolic system. In addition, numerical solution of buoyancy-driven flow is a more difficult problem than forced convection because it includes two very different time scales—both the convective and thermal conductive equilibration times.(Thompson, Leaf et al. 1988) The problem becomes more stiff.

Those CFD solution programs that include buoyancy use some specified combination of the temperature and its normal derivative on the boundary surfaces as a fixed boundary condition for the solution of the flow, pressure and temperature fields in the fluid (i.e., air). Where radiative interchanges among surfaces have been included the usual approach has been to use a separate radiation solver to calculate surface temperatures, based on assumed values of the convective coefficients. These temperatures are then used to solve the CFD problem, which yields new values of the convective coefficients, and the two calculations are iterated until a consistent set of temperatures is reached. This method is likely to be most successful when the flow is dominated by forced convection, since then the dependence of the convective coefficients on the surface temperatures is likely to be small. When buoyancy-driven flow is significant or predominant the method is likely to be inefficient, because small changes in temperature cause large changes in

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flow, so that one spends a great deal of effort producing CFD solutions that are subsequently discarded.

The problem is likely to become still more stiff when the true surface boundary conditions are applied, because the correct coupling to the building structure and equipment introduces a whole range of new time constants. While the long time constant intrinsic to the entire building can probably be dealt with by some form of quasistatic approximation, the time constant of the thermal mass making up the boundary walls will certainly affect the problem. In addition there will be the time constants resulting from the response of HVAC and other building equipment to the state of the interior air (e.g., temperature). The latter will in fact be a subject of great interest for designing better control systems.

From this discussion we can conclude that the present state of the art in CFD calculations is quite far from what is required for a realistic building interior model, and that a focused research effort will be required to reach that goal. Work pursued in other areas of CFD research will not automatically solve the necessary problems, nor is it guaranteed that a straightforward application of techniques developed elsewhere will provide the solution here.

Initial Design Decisions and Project Plan

An initial survey of the literature indicated that CFD calculations with a k-ε turbulence model are presently being applied to large buildings, (Kato, Murakami et al. 1995) turbulence calculations with a variety of models are being researched (Murakami, Mochida et al. 1996; Xu and Chen 1998) and CFD calculation modules are beginning to be included in building simulation codes. (Negrão 1995) This indicated that our research should begin with a CFD calculation having the capability of including a two-equation turbulence model. Initially this calculation would use fixed-temperature boundary conditions, with inclusion of the correct conditions a subject of research. Other desirable features of the calculation should be

- Expandability to large buildings and complex geometries
- Design for easy geometry modification
- Efficient solution method

These requirements immediately pointed up necessary design compromises between the construction of the numerical mesh for a solution and the efficiency of the solver. For complex geometries either a block structured or an unstructured mesh is typically used; however, geometry modifications in a block structured mesh are difficult, while an unstructured mesh has a high computational overhead (related to sorting out the mesh geometry) that makes solvers less efficient than for structured meshes.

Our provisional solution to this conundrum was to focus on the composite (or overset) grid technique. In this method the computational space is filled with a simple basic mesh (such as a structured Cartesian grid) into which localized minor grids are inserted. Holes are cut in the basic mesh where it is covered by the minor grids, and the solution is analytically continued between the major and minor grids. The minor grids may be curvilinear, and are constructed and inserted to allow local adaptation to geometrical complexities. This method is frequently used to accommodate problems with moving boundaries (e.g., turbine blades in a jet engine), a feature which will not be necessary in buildings applications unless one begins to model the effects of moving occupants. While this may be a possible application, it is not an immediate one. Other aspects of the method, however, appear well suited to buildings.

Building spaces begin as simple geometric solid shapes (usually parallelepipeds) and acquire geometric complexity through the addition of detailing (mainly at surfaces and openings to other

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spaces) and objects within the space (e.g., furniture, office partitions). Reconfigurability of spaces is a strong trend in commercial building design. Near any surface the air is capable of forming a boundary layer flow, the simulation of which requires a high mesh resolution along the surface normal. If the building space is filled with a simple mesh matching its basic geometry and minor meshes are attached to surfaces and objects, then the same computational techniques that allow the easy representation of a moving part also allow the easy assembly of a building mesh from its components. This matches the highly modular way that buildings are designed and constructed.

This method should be relatively computationally efficient, since complexities of the mesh (and the attendant computational/bookkeeping burden) are limited to those places where the problem requires them (either because of the geometry or the flow characteristics). Where needed, one could exercise complete freedom in the definition of minor grids, so that not only curvilinear grids, but also desirable features of adaptive or unstructured meshing techniques could be incorporated into the method.
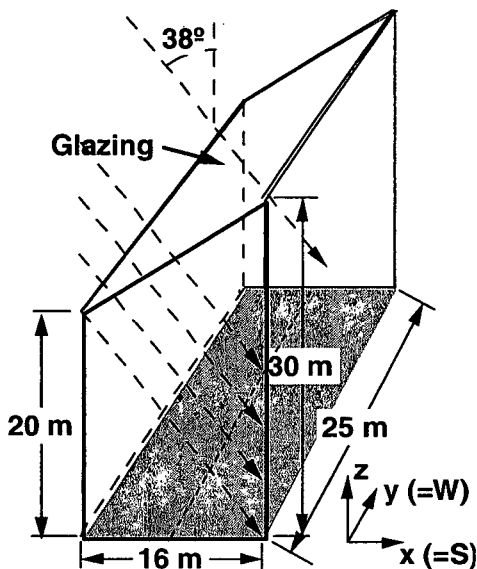

Figure 3. A simple atrium shape defined to serve as an initial test problem. The dashed arrows represent incident sunshine.

An added bonus of this approach is that it adapts well to a systematic, step-by-step approach to the problem. One can begin with simple geometries filled by a single grid, next add planar boundary surface minor grids, and then proceed to more complex details and interior objects, each with its associated minor grid. At each stage the set of worked-out object/grid combinations becomes a library of components that can be used to assemble building interior models at a given level of complexity.

Having chosen a design strategy, we next chose a target problem to serve as an initial goal in developing the model. We picked a simple conceptual atrium, shown in Figure 3. This choice guarantees that at the outset our model must handle large Rayleigh numbers and tilted surfaces, both necessary features in a realistic interior building model. Our plan is then as follows: (1) We first model this problem with conventional state-of-the-art CFD, utilizing fixed-surface temperature boundary conditions. For daytime summer conditions we mock up the solar radiation by assuming reasonable temperatures for the glazed roof and the irradiated wall. For nighttime winter conditions we assume a cold roof. (2) Next, we add a ducting system and the associated flow and pressure boundary conditions to the problem. (3) We add a long-wave radiation exchange model and replace the known-temperature boundary conditions with a net heat balance at the surface (assuming adiabatic walls). (4) We add a solar radiation model (with appropriate interreflections), and include this in the net heat balance at the surfaces. (5) We add thermal mass and heat transfer properties to the envelope and make the problem transient, driven by exterior solar radiation and temperature. (6) Finally, we expand this model to additional parts of a hypothetical building, either through CFD modeling of connected spaces and/or linking our model to a more conventional building simulation model.

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At any stage in the plan, once we have a functioning model capable of solving the model problem we would begin work to test whether the solutions are physically realistic. We could begin this effort utilizing our Mobile Window Thermal Test (MoWiTT) Facility, which has well-controlled rooms measuring 2.4 m X 3.0 m X 2.4 m. This facility would be most useful for testing in stages (3) through (5) for small spaces. For large or empty spaces comparisons with published benchmarks or measurements or via collaboration would be pursued.

Selecting a CFD Code

Implicit in our initial design choices is the intention of focusing our work on buildings, not on CFD techniques. We do not seek to develop a *de novo* CFD code (a daunting prospect in any case). Rather, we wish to adapt the present state of the art to our building problem as expeditiously as possible. This has been an element in our choice of solution strategy. We do not maintain above that in principle unstructured grid methods cannot be made efficient enough, nor adaptive-grid codes flexible enough, to handle building problems. Rather, as of the beginning of this project, these were still areas of active CFD research, while the overset-grid method was relatively well developed. Accordingly, we proceeded to examine ways of most expediently bringing the state of the art in CFD to bear on our test problem.

Commercial CFD Codes vs. In-house Development

An immediate and obvious question is whether it would not be most expedient to utilize a general-propose commercial CFD code, given the availability of numerous products with few advertised restrictions on their applicability. In fact, this approach would certainly be the quickest way to make progress on stage (1), and could be validly used to explore questions such as the nature of the flow solution and the consequences of the choice of turbulence model. We contacted Fluent and Flowmerics in this regard, as well as reviewing project literature for a number of other codes. However, none of the present commercial codes seeks to determine the boundary layer film coefficients or implement the detailed net heat balance boundary condition at surfaces. There is no route for proceeding to the other stages of the project plan without engaging in detailed collaborative code development. We found no CFD code supplier interested in going beyond a simple commercial licensing arrangement.

This is not surprising, given the uncertainty both in the research outcome of this effort and in its market potential. One company we contacted had developed a product aimed at HVAC design and experienced disappointing market response. It is first necessary to investigate whether this modeling is feasible and whether it yields economically attractive opportunities for energy-efficient building design. Only when the answer to these questions is known to be favorable would one expect interest in commercial CFD development in this direction.

To proceed from steps (1) toward (5), therefore, would require some in-house code development. Since project resources were insufficient to support a parallel effort of research within step (1) using commercial CFD code, we turned to the question of acquiring a source code with which to begin.

Survey of Available Public-Domain Codes

We searched for state-of-the-art public domain CFD codes that utilized the overset grid technique or might otherwise be adaptable to building problems.

TEACH/ESP

One interesting development is that the CFD instructional program TEACH-2E (Gosman and Ideriah 1976) has been incorporated as a modeling element in the European building simulation

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model ESP, (Clarke 1985) and has been subsequently expanded to 3D. (Negrão 1995; Clarke, Dempster et al. 1997) TEACH-2E is an implementation of the SIMPLE algorithm (Caretto, Gosman et al. 1972). Since it is a 2-dimensional calculation, TEACH-2E did not appear to be an attractive candidate for a CFD code, but the work on connecting the CFD code with ESP is extremely interesting for step (5). We established communication with the ESP group and plan to collaborate.

GasFlow

One of the earliest programs considered was GASFLOW. (Travis, Lam et al. 1994) Consideration of this code represented a deviation from the project strategy, since GASFLOW does not use an overset grid approach. We had learned, however, that a DOE review (Spore, Boyac et al. 1996) had concluded that it was the best code for assessing the transport of nuclear reactor leakage products within structures, and that it was designed to model buildings. These advantages made it worth examining.

When we obtained a copy of the DOE review, we found that it had been extremely narrow in its focus, and that GASFLOW was the only one of the programs considered that performed a CFD calculation, the others treating essentially networks of well-mixed control volumes. This made the review's conclusions less persuasive.

GASFLOW uses a linearized ICDd-ALE solution method. It builds its model using a Cartesian grid that can be independently block-structured in each coordinate. Within a given block it allows unidirectional quadratic variation of mesh size. This type of mesh definition essentially requires that the mesh blocks be hand-designed to fit the problem, and for a 3D structure of any complexity the mesh becomes inefficient, since small mesh sizes needed in one location are carried along the coordinate axes to locations where they are unnecessary. Heat transfer into or out of surfaces is assumed one-dimensional and radiative heat transfer is simplified. Here and in many other places approximations and simplifications are made that are appropriate to the code's original purpose—namely, study of hydrogen fires and other accident conditions in nuclear containment vessels—but that have little to do with normal building interiors.

We concluded that GASFLOW is inappropriate for use as a starting point in constructing a building interior model. It is a program originally designed for specific applications, and simplifying assumptions appropriate to the original applications are made in numerous places throughout. To make the program suitable for studying building interiors one would need to replace these assumptions and replace the mesh generation strategy with one that is more economical for a large complex building. This would leave the solver as the only original piece of code, and since there are better solution methods there is little motivation for choosing this route.

Overture

The Overture system (Brown and Henshaw 1996) is an outgrowth of the FORTRAN-based program CMPGRID developed at Los Alamos National Laboratory, which was one of the state-of-the-art implementations of CFD solutions on overset grids. CMPGRID proved too difficult to maintain and has been discontinued; Overture, which is written in C++, is its replacement.

In many ways, Overture would have been the ideal tool for this project, since it is a "toolbox" approach that provides flexible CFD modules that work within a composite-grid approach without making assumptions about the global structure of the problem. It incorporates some highly efficient techniques, such as multigrid solvers for elliptic equations, and is designed to facilitate efficient parallel computation on a variety of computer platforms. However, at the time

this project began the construction of Overture was incomplete in several crucial respects. First, there was no released incompressible Navier-Stokes solver. Second, C++ compilers were much less successful at code optimization, resulting in much less efficient execution code than comparable FORTRAN implementations. Third, (which was less crucial for our immediate purposes) the implementation of the parallel computation scheme was incomplete.

These difficulties made the Overture code inappropriate for near-term use, but it remains a development to be tracked.

LBNL Codes

Two possible sources of CFD codes at LBNL were investigated. We met with John Bell to discuss codes developed by his combustion research group. They did not have a code solving simple buoyancy-driven convection available, and our conclusion was that attempting to use what was available would require more program development than was feasible. A second option was CONVEC2, a 2-D implementation of the SIMPLE algorithm used a number of years ago for buoyancy-driven convection problems. (Gadgil 1980) We concluded that here also too much development effort would be required to bring the program up to date and adapt it to the current problem.

INS3D

The Incompressible Navier-Stokes code, INS3D, (Rogers and Kwak 1988; Rogers and Kwak 1988; Rogers and Kwak 1991; Rogers 1995) was briefly considered. The supported version of INS3D does not solve the heat equation and thus was not suitable to the building model problem.

Overflow

OVERFLOW, (Buning, Jespersen et al. 1997) developed at NASA Ames Laboratory, is a compressible-flow solver with a preconditioning algorithm (Jespersen, Pulliam et al. 1997) to improve the solver properties for low Mach number flows, (Turkel 1987; Leer, Lee et al. 1991; Choi and Merkle 1993) and buoyancy terms have recently been added. As a feasibility study (Olsen and Banks 1998) we examined its behavior for a simple cubic geometry where the flow was driven entirely by buoyancy effects. It proved difficult to achieve convergence on the problem with the version of the code available at that time, and this line of investigation was not pursued further.

Research Codes from UC Davis

A set of research codes (Dwyer 1989; Nirschl, Dwyer et al. 1995; Dwyer and Stapf 1996) developed jointly at the University of California, Davis, the University of Munich, and Daimler-Benz Research Laboratories, Stuttgart, Germany, (termed the "UC Davis code") uses an overset grid scheme to solve the variable-density fluid dynamics equations. This code was developed to study reacting fuel droplets and had been originally written to include buoyancy. The code included a capability for handling chemically reacting flows, which is not needed in a building model. However, this capability did not appear to have been implemented in a way that either introduced inapplicable assumptions or significantly slowed down the solution when it was not used. The program uses a structured Cartesian mesh with overset minor grids, the basic structure we wished to use. It used an Alternating Direction Implicit (ADI) solution method, which is relatively modern and fast. In short, while not without artifacts that would need to be removed, it appeared to form a workable basis with which to begin. It would enable us to begin on step (1), with a reasonable investment of code development effort, while providing the correct structure for proceeding to subsequent steps in the plan.

Code Development

We utilized the UC Davis code as a basis for a modified code, CHIFLOW, to be used on the model problem. The minor grids, which had been programmed into the code, were removed and a more flexible definition created by adding an interface to the overset grid domain continuity routine PEGSUS. (Suhs and Tramel 1991) Numerical viscosity was added to the laminar code in order to obtain convergence for the full-size atrium using a reasonable mesh size. A two-equation turbulence model was also added.

RESULTS

Benchmark tests of the calculation were made by solving a 2D rectangular "double glazing" problem for a square enclosure. Comparison of these calculations with a published numerical solution for the same problem (Newell and Schmidt 1970) showed qualitatively correct flow and temperature patterns. Repeated solutions of the problem with different grid mesh sizes indicated that for sufficiently fine mesh sizes the solution did not depend on the mesh size, and the Nusselt number converged to a unique value. The issue of whether this value is physically correct was not pursued at this point, since it pertains to the details of the near-wall solution rather than the overall behavior of the solver. These calculations were carried out on a region of very small overall dimensions, in order to guarantee a laminar solution without use of numerical viscosity. The solver showed the "stalling" behavior expectable of a relaxation solution without special provisions (such as multigrid) for reducing error terms with slow spatial variation.

Next the laminar code with numerical viscosity was applied to the full-size atrium problem. This application represented the very beginnings of step (1), the solution on the base grid before the addition of any minor grids. Since the addition of minor grids is planned to handle both the near-wall grids for fitting surface boundary conditions and departures from rectangular parallelepiped shapes, such as the slanted atrium roof, one could not make a solution only for the major grid without making compromises. Here we used a body-fitted space-filling mesh with increasing mesh density near the surfaces. This grid is shown in Figure 4. Since CHIFLOW handles curvilinear grids, use of this mesh did not require any special provisions (although the solution may be slower than on a simple Cartesian major grid).
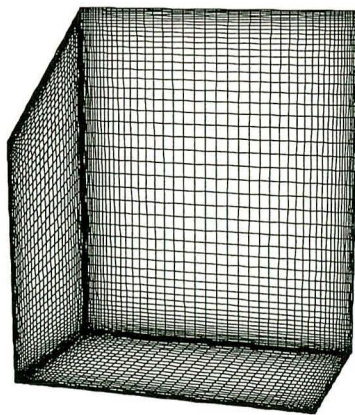

Figure 4. Computational grid used for the atrium in Figure 3. Note that the grid is rotated by 90° from the diagram in Figure 3, so that the y-axis points horizontally and to the right.

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The behavior of the code was first checked by running the 2D square enclosure problem on a skewed curvilinear grid. On this problem the Nusselt number obtained was within 2% of that obtained with an orthogonal Cartesian grid. Convergence was indeed slower, with the residual after a fixed number of iterations in the curvilinear case approximately twice as large as for the orthogonal Cartesian grid.

CHIFLOW was then used to model the atrium interior for simulated nighttime winter conditions in an unoccupied atrium. The walls and floor were assumed to be interior to the building and were assigned a temperature of 16 °C, modeling a nighttime temperature setback. The roof was assumed to be double-glazing and to have an interior surface temperature of 10.4 °C, which would be reasonable for an outdoor air temperature of 0° C. These were taken as fixed-surface-temperature boundary conditions for CHIFLOW. These conditions were chosen because the next planned step is to simulate conditioning of the occupied lower portion of the atrium by introducing warm airflow through ducts.

The solution produced a flow pattern in the shorter central plane of the atrium rather similar to what one might expect on the basis of the 2D double glazing solution. Figure 5 shows a circulating flow initiated by the cold roof; the corresponding temperature field is shown in Figure 6. The central plane parallel to the long dimension of the atrium shows a more complicated flow pattern, Figure 7, with downwelling of air in the center and upward motion along the walls. Figure 8 gives the corresponding temperature field in this plane. In Figures 9 and 10, two views of one-half of the atrium show the trajectories of hypothetical tracer particles released into the flow at several points; these figures show that the flow pattern is essentially 3-dimensional.
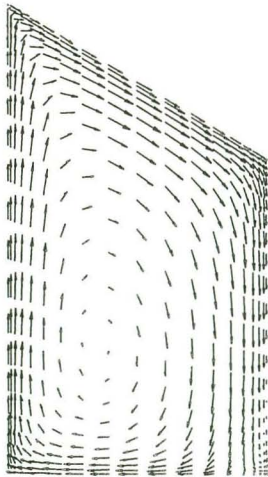

Figure 5. Velocity vectors in the x-z plane at the center of the atrium. Note that here the y axis points into the plane of the paper and the x axis is horizontal pointing to the left.
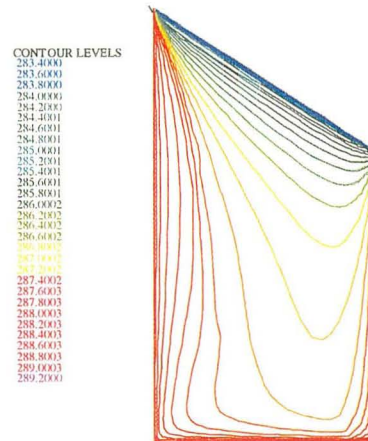

Figure 6. Temperature contour plot in the central x-z plane of the atrium.
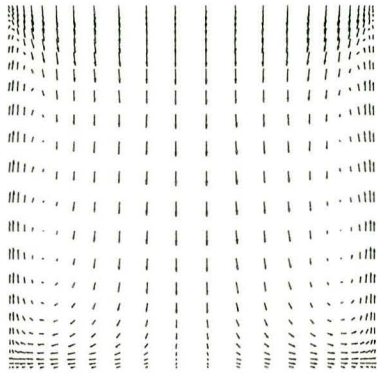
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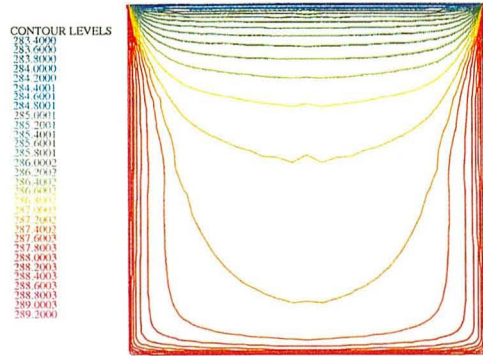Figure 7. Velocity vectors in the y-z plane at the center of the atrium.

Figure 8. Temperature contour plot in the central y-z plane of the atrium. Figure 8 gives the corresponding temperature field in this plane. In Figures 9 and 10, two views of one-half of the atrium show the trajectories of hypothetical tracer particles released into the flow at several points; these figures show that the flow pattern is essentially 3-dimensional.
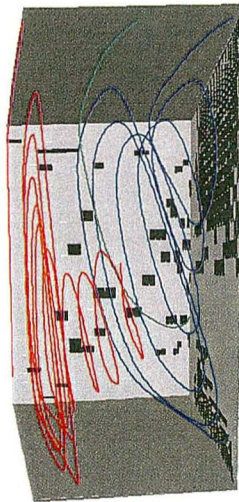

Figure 9. Trajectories of individual fluid elements in the atrium. Half of the atrium is shown, as viewed through the central x-z plane. Viewing angle is nearly normal to the x-z plane, i.e., the viewer is looking in nearly the positive y direction. The x-axis points horizontally to the right. At a given time three tracer particles are released near the highest point of the ceiling (which is viewed in perspective from the inside) and their subsequent trajectories shown. One particle (red) is in the central x-z plane, a second (blue) is near the far wall of the atrium, and the third (green) is midway between. Initial x and z values of all three particles are the same.
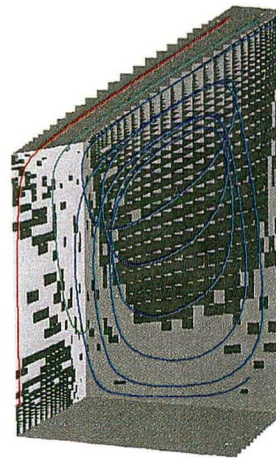

Figure 10. Trajectories of individual fluid elements in the atrium. The same half of the atrium as shown in Figure 9 is viewed, but this time the viewing angle is nearly parallel to the central x-z plane, which forms the left boundary of the figure. In addition to the three fluid element trajectories shown in Figure 9, an additional trajectory (red, with complicated path) is shown for a fluid element that is originally near the center of the half of the atrium shown [i.e., initial (x,y,z)=(0,0,15m), where the origin of the coordinate system is taken at the center of the floor of the atrium in Figure 3.

This solution represents a reasonable qualitative picture of flow and temperature, but it is not the correct one because the near-wall modeling is not yet correct, turbulence is not included and the assumed boundary conditions are artificial. Only when all of the steps 1 through 6 have been carried out (useful results may be obtained at step 4) will one have the correct boundary conditions, and therefore possibly a quantitatively correct solution. But even this preliminary solution provides some useful insights. First, the 3-dimensional nature of the flow, as shown in Figure 10, is very unlikely to become less 3-dimensional in a more detailed calculation (the contrary is more probable). One frequently sees in the literature 2-dimensional CFD calculations done in a symmetry plane and presented with the assumption that the flow and temperature patterns calculated persist in the 3-dimensional case until close to the "edge region" in the neglected dimension. Figure 10 indicates that the third dimension alters the flow as soon as one moves off the symmetry plane (the central x-z plane in Figures 9 and 10).

Second, one can see how little a reasonable-seeming flow and temperature pattern guarantee the correctness of the calculation. In Figure 5, one could expect that inclusion of turbulence in the calculation might cause separation and the formation of downward plumes at the ceiling, at least at some ceiling temperature. A radiant interchange calculation and detailed modeling of the near-wall region would produce different surface temperature and convective film coefficients from those assumed, which in turn might alter the flow pattern. In particular, radiant interchange between the ceiling and the wall at left in Figure 5 would tend to produce a wall surface temperature that decreased with height; at some point this should begin to cause a recirculating cell in the wall flow. All of the changes in flow and radiation exchanges would alter both the surface temperatures and the convective coefficients, which implies an altered heat flow through the envelope surfaces and hence a different load on the space. In short, while this proof-of-concept calculation (which was not intended to be physically correct) produced flows that appear reasonable, none of the reasonable-appearing features of the calculation can be taken as an indicator that the result is physically correct, or to give an estimate of how close or far the model result is from the true solution.

Nevertheless, having a solution before us does give concreteness to the question of applications, and it is useful to consider what new information would be provided to the building designer if the solution were correct.

The local temperature and airflow distributions, taken together with the radiant temperature that can be calculated for any given location from the surface temperatures, would allow one to evaluate local thermal comfort. For this atrium the first problem would be to determine the duct locations and air flows needed to produce acceptable comfort conditions in the occupied zone, and to evaluate the energy requirements of alternative strategies for supplying this. Forced-air circulation in the occupied zone verses displacement ventilation are examples of such alternative strategies. In addition, airflow and temperature distributions would allow the calculation of pollutant, odor and moisture conditions, as well as particulate deposition and the potential for condensation. The time delays between the onset of conditions at a localized control sensor that cause some action by the HVAC system (e.g., a change in heating or fan speed) and the results of the control action for various locations in the space could also be determined. Thus, a correct building interior model would provide a number of important pieces of information not presently available to the designer.

CONCLUSIONS

In order to achieve in a timely manner the large energy and dollar savings technically possible through improvements in building energy efficiency, it will be necessary to solve the problem of

design failure risk. The most economical method of doing this would be to learn to calculate building performance with sufficient detail, accuracy and reliability to avoid design failure. Existing building simulation models (BSM) are a large step in this direction, but are still not capable of this level of modeling. Developments in computational fluid dynamics (CFD) techniques now allow one to construct a road map from present BSM's to a complete building physical model. The most useful first step is a building interior model (BIM) that would allow prediction of local conditions affecting occupant health and comfort.

To provide reliable prediction a BIM must incorporate the correct physical boundary conditions on a building interior. Doing so raises a number of specific technical problems and research questions. The solution of these within a context useful for building research and design is not likely to result from other research on CFD, which is directed toward the solution of different types of problems. A six-step plan for incorporating the correct boundary conditions within the context of the model problem of a large atrium has been outlined.

A promising strategy for constructing a BIM is the overset grid technique for representing a building space in a CFD calculation. This technique promises to adapt well to building design and allows a step-by-step approach. A state-of-the-art CFD computer code using this technique has been adapted to the problem and can form the departure point for this research.

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