Title

Support to DHS Chemical Detection Field Testing and Countermeasures Studies: Report to Sponsors

Authors

Sohn, Michael
Black, Douglas
Delp, William

Publication Date

2011-09-01

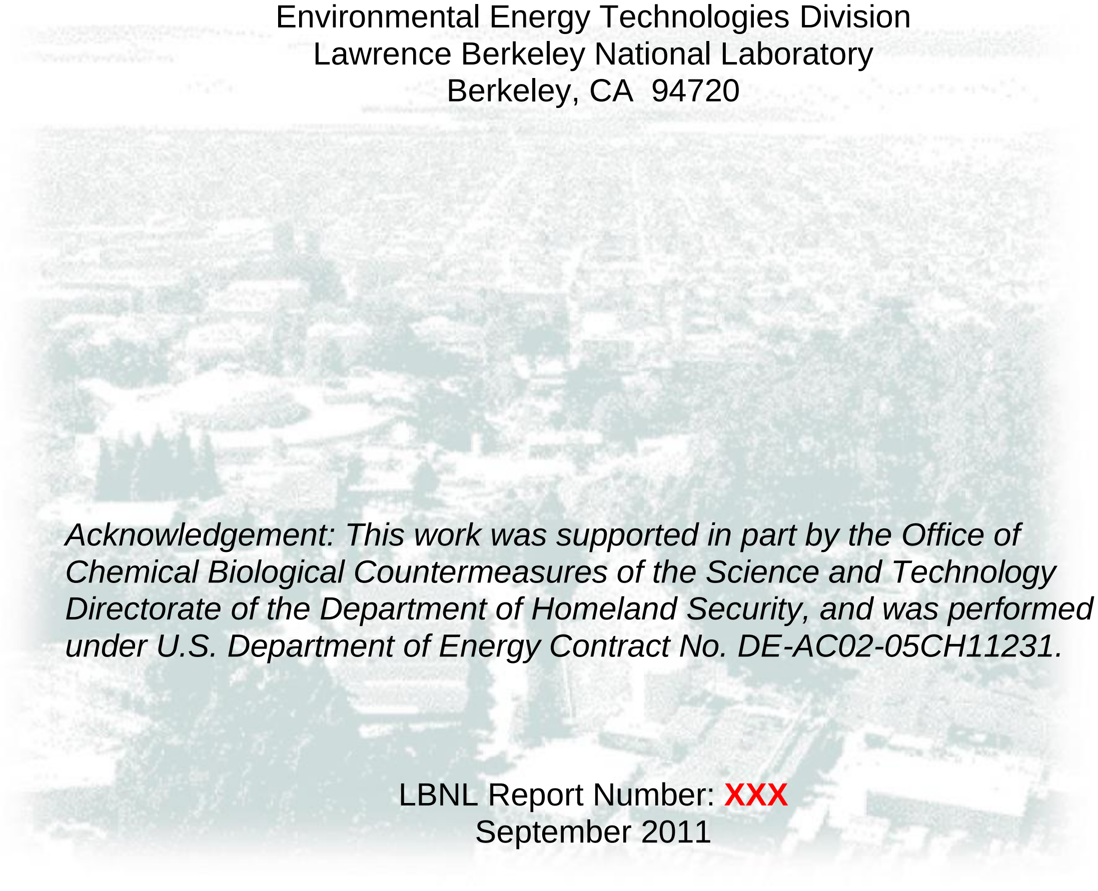
ERNEST ORLANDO LAWRENCE
BERKELEY NATIONAL LABORATORY

Support to DHS Chemical Detection Field Testing and Countermeasures Studies: Report to Sponsors

Final Report to Sponsor

Version 1.1

Michael D. Sohn, Douglas R. Black, William W. Delp
Indoor Environment Department
Environmental Energy Technologies Division
Lawrence Berkeley National Laboratory
Berkeley, CA 94720



Acknowledgement: This work was supported in part by the Office of Chemical Biological Countermeasures of the Science and Technology Directorate of the Department of Homeland Security, and was performed under U.S. Department of Energy Contract No. DE-AC02-05CH11231.

LBNL Report Number: XXX
September 2011

Table of Contents

Executive summary

This document reports on work that Lawrence Berkeley National Laboratory performed to support the Department of Homeland Security's testing of ARFCAM and LACIS systems. In the sections that follow, LBNL lists the scope of work, field analyses conducted, and preliminary results.

LBNL developed a model of the Port Gaston building at the Nevada Test Site and calibrated it using data from field experiments, both blower door and tracer gas tests. Model development and comparison to data show very good agreement. The model was developed to (1) support the interpretation of data from field trials performed by Signature Science LLC, (2) support the placement of sampler equipment, and (3) predict if meteorological differences between the Wet-Run/Dry-Run and the Hot-Run might adversely affect the development of the Hot Run Test Plan. LBNL reported its findings on each task to the experiment team at scheduled planning meetings. In the end, we note that the model was used limitedly because the data from the Wet-Run/Dry Run were if such high quality.

Lastly, LBNL conducted a research experiment at the end of the Wet-Run/Dry-Run to study if, and to what degree, specific TICs sorb and desorb on indoor surfaces. We found that several of the TICs either sorb onto surfaces or are lost through chemical reactions. These findings may have important implications on determining sheltering-in-place concepts of operation.

1. Background

The US Department of Homeland Security (DHS) Chemical Detection Program aims to enhance and coordinate the Nation’s capability to anticipate, prevent, protect, respond to and recover from chemical threat attacks through innovative research, development, and transition of capabilities. Areas of interest include: (1) development of a National chemical defense architecture; (2) chemical characterization, detection, and interdiction; (3) rapid recovery and decontamination activities; (4) increased understanding of chemical source attribution and forensics; and (5) processes to minimize effects of chemical attacks.

The Detection Program supports technology development for warning and notification of a chemical threat release including technologies needed by responder personnel to conduct surveys of potentially contaminated scenes. Target performance characteristics for detectors will be established for different detector applications, and a process to certify that candidate technologies perform as specified will be defined. The program will work toward the development of technologies that can, in a single package, sense chemical hazards of possible terrorist use as well as more commonly monitored chemicals at costs that will support true dual-use application. Developing such a capability requires a leap forward in technology; research toward that end is embedded across detection technical milestones.

DHS presently is developing detect-to-warn facility monitors and hand-held incident detectors. These projects were initiated under Broad Area Announcement RA 03-01, Technical Topic Areas (TTAs) 3 and 4 (http://www.hsarpabaa.com/). Detectors that have successfully completed Phase I and II of these projects will be tested in realistic field environments during Phase III.

The ARFCAM (Autonomous Rapid Chemical Agent Monitor, RA 03-01, TTA-3) Project will develop a "detect-to-warn" system capable of monitoring facilities for the presence of CWAs (Chemical Warfare Agents) and high-priority TICs (Toxic Industrial Chemicals). This system will continuously and autonomously monitor, and be capable of detecting and identifying these chemicals with a response time that provides sufficient warning to enable effective response measures such as active management of air flows, evacuation, and notification of responders.

The LACIS (Lightweight Autonomous Chemical Identification System, RA 03-01, TTA-4) Project will develop, field-test, and transition to commercialization a next-generation, hand portable, detection and identification system for chemical vapor hazards such as CWAs and high-priority TICs. This detection system will provide first responders with an accurate, near real-time analysis of chemical hazards and will help responders determine what level of personal protective equipment would be required at an incident scene.

Lawrence Berkeley National Laboratory is supporting the field testing of ARFCAM and LACIS systems. In the sections that follow, LBNL lists the scope of work, field analyses performed, and results. The work is performed pursuant to the prime contract between the Department of Energy (DOE) and LBNL for research, testing, evaluation, and/or development activities and pursuant to Section 309(a)(1)(c) of the Homeland Security Act of 2002 (Public Law 107-296) which authorizes DHS to task the DOE National Laboratories on a "work for others" basis.

2. Scope of work

LBNL reports on two tasks to support the testing of prototype chemical detectors developed under the ARFCAM and LACIS Projects at the Port Gaston building at the Nevada Test Site (NTS). Task 1 is the development and testing of a CONTAM-based model of the Port Gaston building at the Nevada Test Site (NTS), and to provide Subject Matter Expert (SME) support. Task 2 is to support the field testing by recommending prototype and ground truth detector placement within the Port Gaston building, and to provide further SME support. Table 1 describes the tasks, dates, and deliverables.

Table 2.1: LBNL statement of work, task description, and deliverables.

Program Element / Project	Major Tasks	Key Milestones and Deliverables
Required time periods are measured from the contract award date		
Task 1: Model Development & Validation and SME Support		
Subtask 1.1: *Develop detailed multi-zone model of Port Gaston building at NTS.* The model will be suitable for predicting various gas release scenarios in the building. LBNL will also exercise the model to simulate the proposed experiments for testing the prototype chemical detectors.	• **1-3 months**: Site visits, team meetings, and review blueprints • **3-6 months:** Develop preliminary model. • **6-9 months:** Update model as needed prior to and after field experiments.	• **9 months**: CONTAM model of building.
Subtask 1.2: *Conduct field and chamber studies, as needed, to verify the performance of the multi-zone model.* Certain building characteristics can	• **1-3 months**: Determine experiment needed, if any. • **3-6 months**: Complete experiments.	• **9 months**: Report on results from experiments.

Program Element / Project	**Major Tasks**	**Key Milestones and Deliverables**
Required time periods are measured from the contract award date		
affect the overall performance of the multi-zone model. LBNL will determine if key building conditions are unknown (e.g., leakages, HVAC performance, flows through complex openings) and conduct various tracer gas and blower door experiments to describe them. LBNL will coordinate such experiments with the NTS and DHS performers.		
Subtask 1.3: *SME support.* LBNL will participate in any pre- and post-experiment meetings. LBNL will help in planning the testing experiments to ensure that data from them will be suitable for analyzing the performance of the prototype chemical detectors. LBNL will also provide briefings on current understanding, and research needs, on building performance and chemical dispersion in buildings.	• **1-15 months**: Provide guidance to DHS, performers, and other interested parties.	• **15 months:** Final report.
Task 2: Field Testing and SME Support		
Subtask 2.1: *Recommend prototype and ground truth placement for field testing at NTS.* LBNL will apply its existing algorithms for sampler placement and sensor data fusion to help place the prototype chemical	• **1-3 months**: Gather performance details on sensor hardware. • **6 months**: Recommend sampler placements.	• **10 months**: Report on optimal sampler placements and comparison to field experiments.

Program Element / Project	Major Tasks	Key Milestones and Deliverables
Required time periods are measured from the contract award date		
detectors. LBNL will work with performers and DHS clients to analyze the performance of the chemical detectors.		
Subtask 2.2: *SME support.* LBNL can serve as an independent review of the results of the detector testing. LBNL will assist DHS in determination of requirements for next generation chemical detectors.	• **1-15 months**: Provide guidance to DHS, performers, and other interested parties.	• **15 months:** Final report.

3. Work completed for Task 1

LBNL conducted field experiments to characterize the airflow patterns in the Port Gaston building and to develop an airflow and pollutant transport model. In this section, we describe the execution and results of the field experiments and the development of the model. The experiment test plan is included in Appendix A of this report.

3.1 Blower door experiments

A “blower-door” experiment is used to determine the tightness of a building envelope. The method is described in ASTM E779. For an individual test, a calibrated fan (or fans) is placed in an exterior doorway using a special frame. The operator then pressurizes (or depressurizes) the building by blowing air into (or out of) the building using the calibrated fan. The resulting pressure difference (inside to outside) and flows are fit to an empirical power law equation:

$$Q = C \cdot sign\left(\Delta P\right) \cdot \left|\Delta P\right|^{n}$$

Where Q is the flow through the blower door [vol/time], C is a flow coefficient; ΔP is the pressure difference; sign(ΔP) is either a positive or negative sign depending on the direction of flow (into or out of the building); and n is a pressure coefficient. In the experiment, the operator measures Q and ΔP to derive C and n. We note that the unit of C is loosely defined because the power law equation is empirically derived; since ΔP has units of pressure, C has units of volume/time divided by pressure raised to the n power.

To reduce the awkwardness of the power law equation, scientists developed a term, called “effective leakage area” (ELA), with units of area:

$$Q = ELA \cdot \sqrt{\frac{2\Delta P}{\rho}}$$

Where ρ is the air density. We can then cast the power law coefficients as an ELA:

$$ELA_r = C \cdot \Delta P_r^{n-0.5} \cdot \sqrt{\frac{\rho}{2}}$$

Where r is some reference pressure difference, such as 4 or 25 Pa.

For the Port Gaston building, the test equipment consisted of Model-3 Minneapolis Blower Doors and an Automated Performance Testing System data collector, both from the Energy Conservatory. The data was imported into Excel and its non-linear solver was used to determine C and n.

The blower door tests were performed on April 16, 2010. The building required three blower door fans to create a 50 Pa pressure difference between the inside and outside. One fan was installed in the West door, and one in each of the two East doors, as shown in Figure 3.1.1.

Figure 3.1.2 shows both the data and example fits of the power law equation to them. The overall effective leakage at 25 Pa, ELA_{25}, was 6,770 cm^2. The data from the experiments are included in the electronic files accompanying this report.

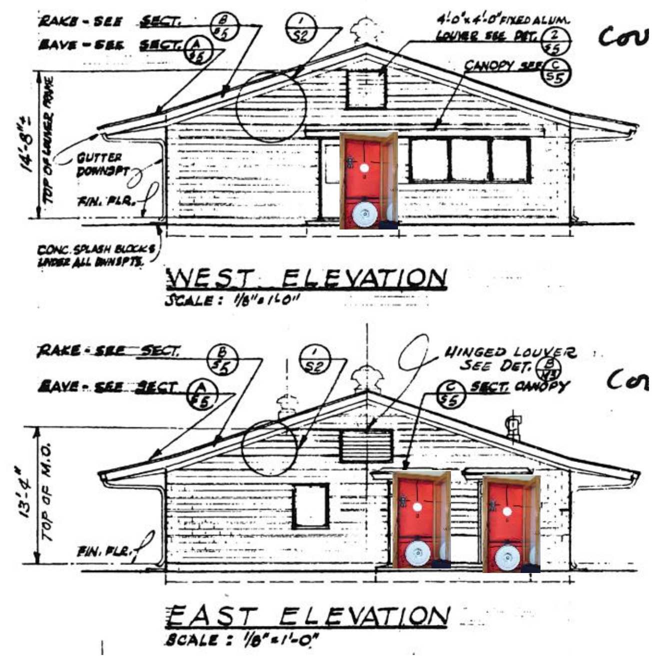


Figure 3.1.1: Location of the three blower door locations shown in red.

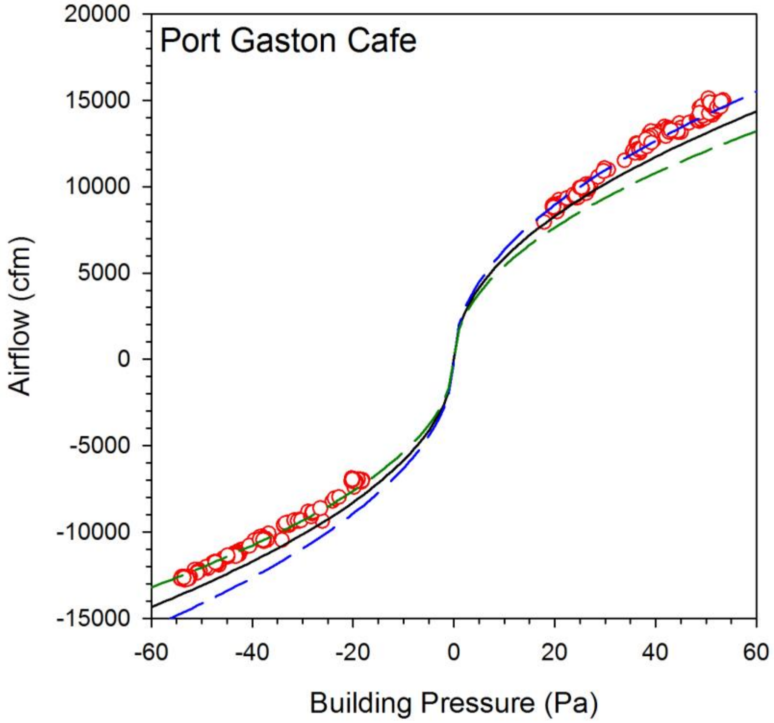


Figure 3.1.2 Data from the blower door experiment. The red circles are the data. The blue dashed line represents the fit using positive pressurization data only, the dashed green line is the fit with the negative pressurization data, and the solid black line is using all of the data.

3.2 Sulfur hexaflouride experiments

Sulfur Hexafluoride (SF_6) is an inert gas used as a conservative tracer in building ventilation studies. On April 15, 2010 LBNL performed SF_6 tracer decay tests at the Port Gaston building. LBNL conducted two morning tests and two afternoon tests. Tests were performed with the HVAC system on and off.

The experiment test plan is included in the Appendix. Briefly, an experiment consisted of releasing SF_6 gas into the HVAC supply plenum for approximately 10 minutes, and recording the indoor concentrations in the building for approximately 120 minutes. For the HVAC-off experiments the HVAC was turned off after the 10 min release of SF_6.

SF_6 measurements were taken using MIRAN SapphIRe SLs from Thermo Scientific at four locations in the building (designated A,B,C, and D on Figure 3.2.1). Figure 3.2.2 shows the indoor SF_6 concentrations as a function of time.

The concentration decay profile was fit to a first-order decay equation:

$$C(t) = C_0 \times e^{-\lambda(t-t_0)}$$

where: C(t) is the concentration at time t [mass/vol], C_0 is the initial concentration [mass/vol], λ is the effective air exchange rate [1/time], and t_0 is the time at the initial concentration. In Figure 3.2.2, with the concentration plotted in log scale, the slope of the lines are λ.

The effective air exchange rate when the HVAC system was operating was approximately 5.5 h^{-1} in the morning and approximately 4.5 h^{-1} in the afternoon. With the HVAC system off, the effective air exchange rate was approximately 0.85 h^{-1} in the morning and 0.65 h^{-1} in the afternoon. During building purge the effective air exchange rate was approximately 20 h^{-1}.

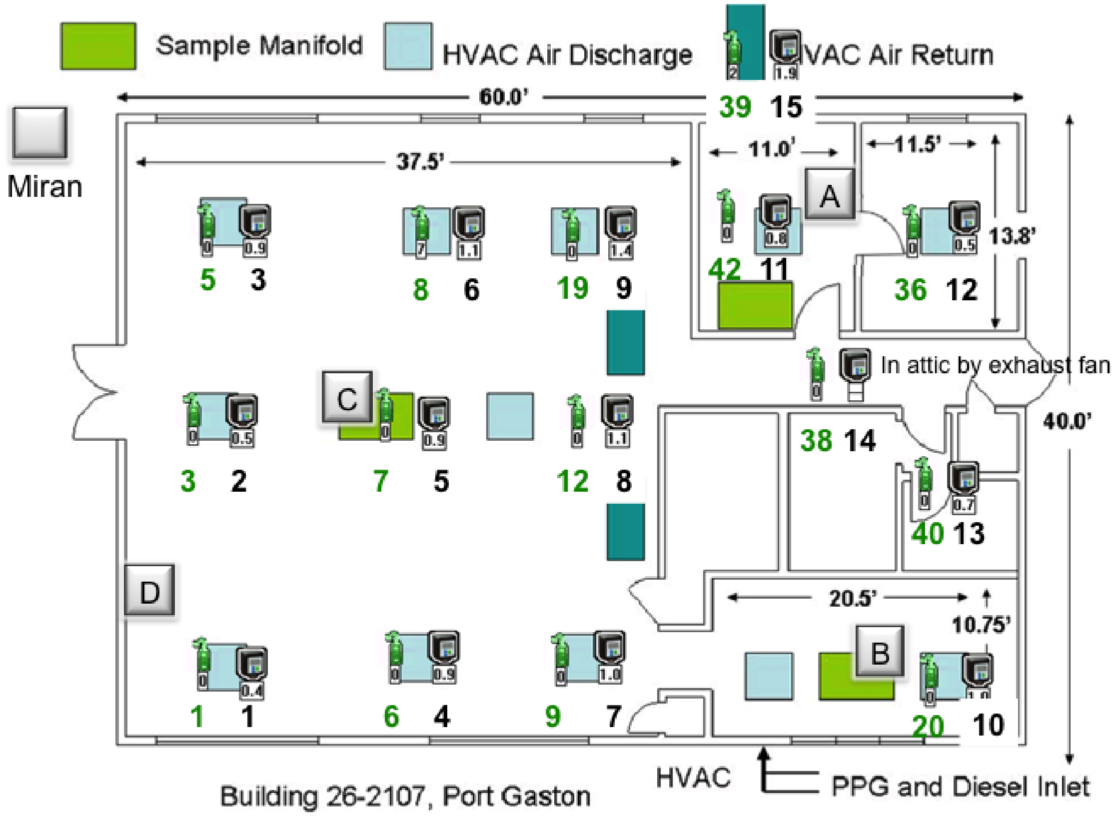


Figure 3.2.1: Floor plan of building, and locations of samplers and HVAC air supplies and returns. Green numbers indicate the location of RAE 3000 photo-ionization detectors (propylene) and black numbers indication the location of Drager 7000 Polytron electro-chemical detectors (TICs). The grey boxes with letters are the location of Miran Sapphire SF_6 analyzers.

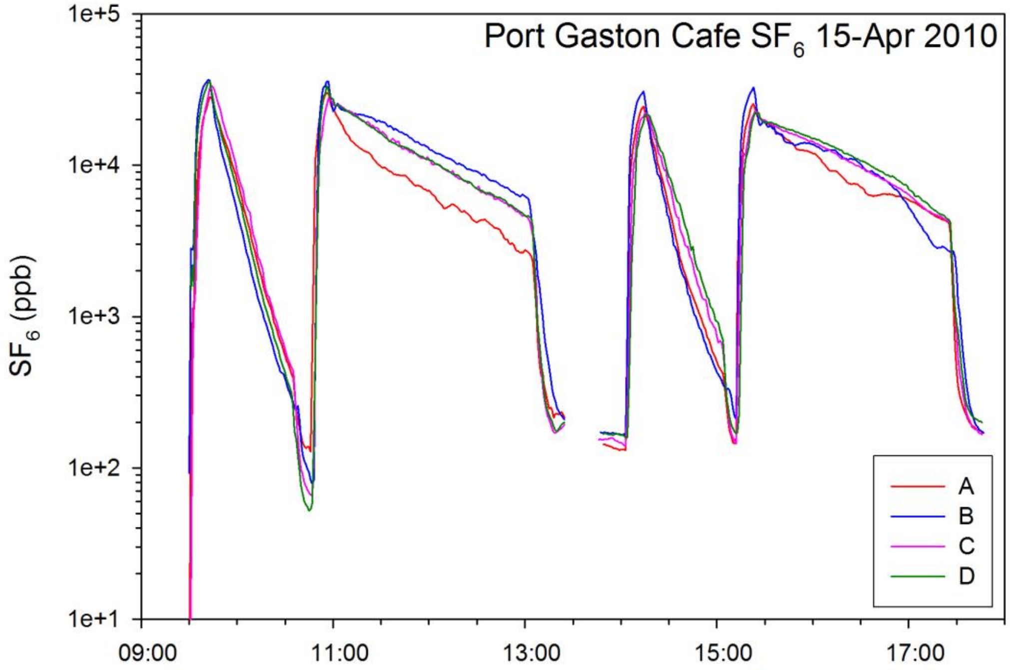


Figure 3.2.2: SF$_6$ experiments conducted on April 15, 2010. Sampler locations A-D are shown in Figure 3.2.1. HVAC was on during 9:00-11:10 and 14:00-15:23. The HVAC was off from 11:10-14:00 and 15:23-17:30. The building purge fans were on at 10:50, 13:00, 15:00, and 17:30.

3.3 COMTAM model of Port Gaston building

LBNL developed an indoor airflow and pollutant transport model of the Port Gaston building using the CONTAM software (NIST, http://www.bfrl.nist.gov/IAQanalysis/). CONTAM uses a multi-zone, well-mixed, model approach to predict airflow and gas transport between rooms or “zones” in the building, and between the indoors and outdoors. The above website details the verification of the code and its use in peer-reviewed journal publications. LBNL has used CONTAM for various homeland security and defense-related studies.

LBNL obtained building and HVAC plans of the Port Gaston building from staff at the Nonproliferation Test and Evaluation Complex (NPTEC) to develop the CONTAM model.

The first step in the model development is to construct a building floor plan and HVAC network in CONTAM. Figure 3.3.1 shows the resulting building model. Each room in the building is represented as a zone in the model. Air can flow between zones through doors, windows, cracks, and ductwork.

Our next step was to calibrate the model to field data. The blower door experiments indicate that the total building leakage under a 25 Pa difference, ELA_{25}, was 6,770 cm^2. The SF_6 experiments indicate that air exchange rates at ambient pressure ranged between 4.5 to 5.5 h^{-1} with the HVAC on, and 0.65 to 0.85 h^{-1} with the HVAC off.

The locations of all leaks in the building are not known so one must iteratively determine how to apportion the leaks throughout the building. Through trial and error, we found that apportioning 85% of the leaks to the attic yielded concentration profiles similar to the results from the SF_6 experiments. LBNL confirmed this apportionment during the site visits and experiments by noting the numerous openings in the attic and only an unconfined “dropped” ceiling separating the attic and occupant floor.

Figure 4.2.1 shows the SF_6 measurements and the model predictions for the main room at the Port Gaston Building on April 15, 2010. When the HVAC is on (9:00-11:10 and 14:00-15:23) the model agrees very well with measurements. When the HVAC is off (11:10-14:00 and 15:23-17:30), the model predicts slightly higher air exchange. Given that ARFCAM and LACIS experiments will be conducted with the HVAC on, we felt that model calibration was suitable for the intended application of the model: sampler placement and evaluation of the Hot Run Test Plan.

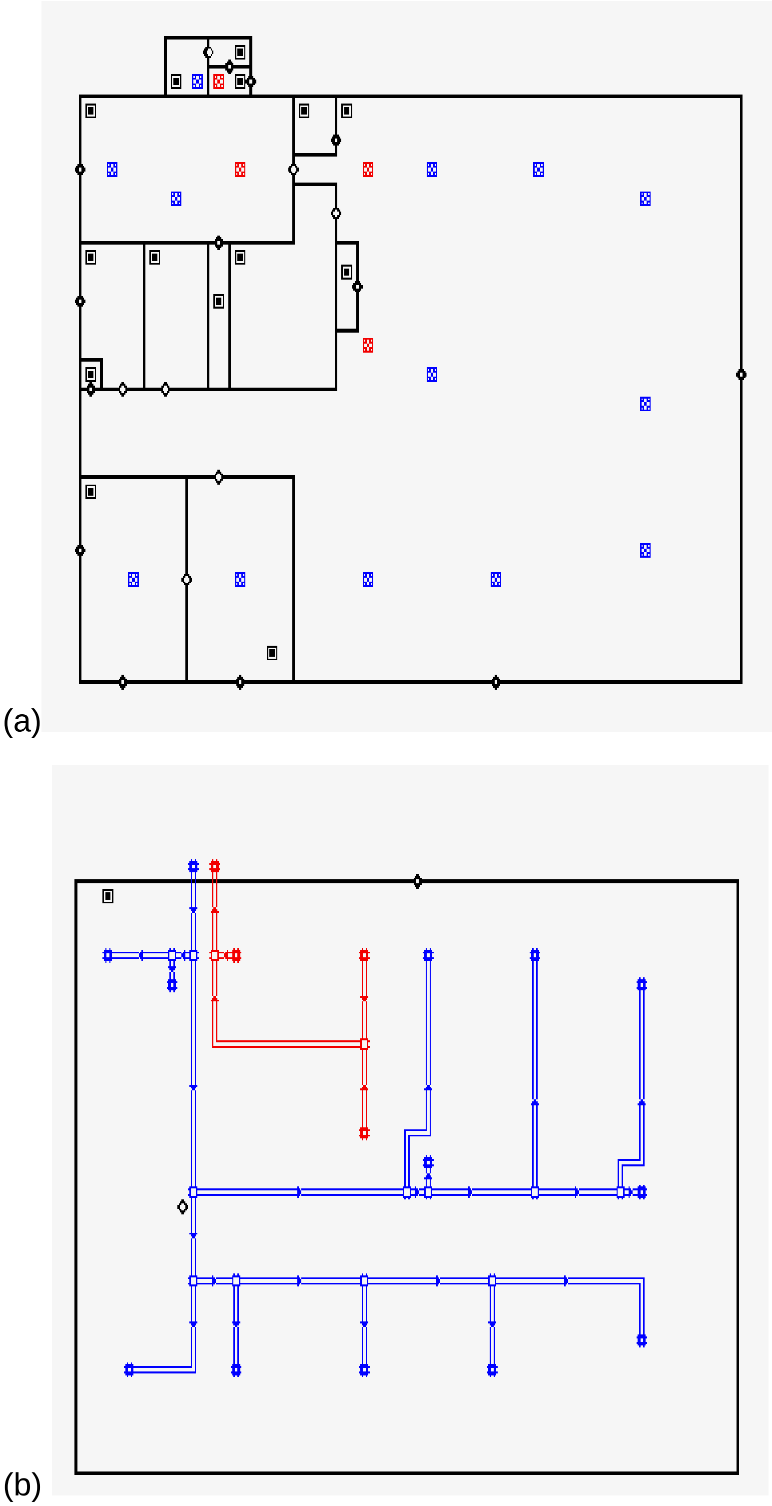


Figure 3.3.1: Schematic of the CONTAM model: (a) main floor and (b) attic. The black lines delineate zones in the model. Blue and red lines represent supply and return ducts, respectively. Blue and red squares are supply and return registers, respectively.

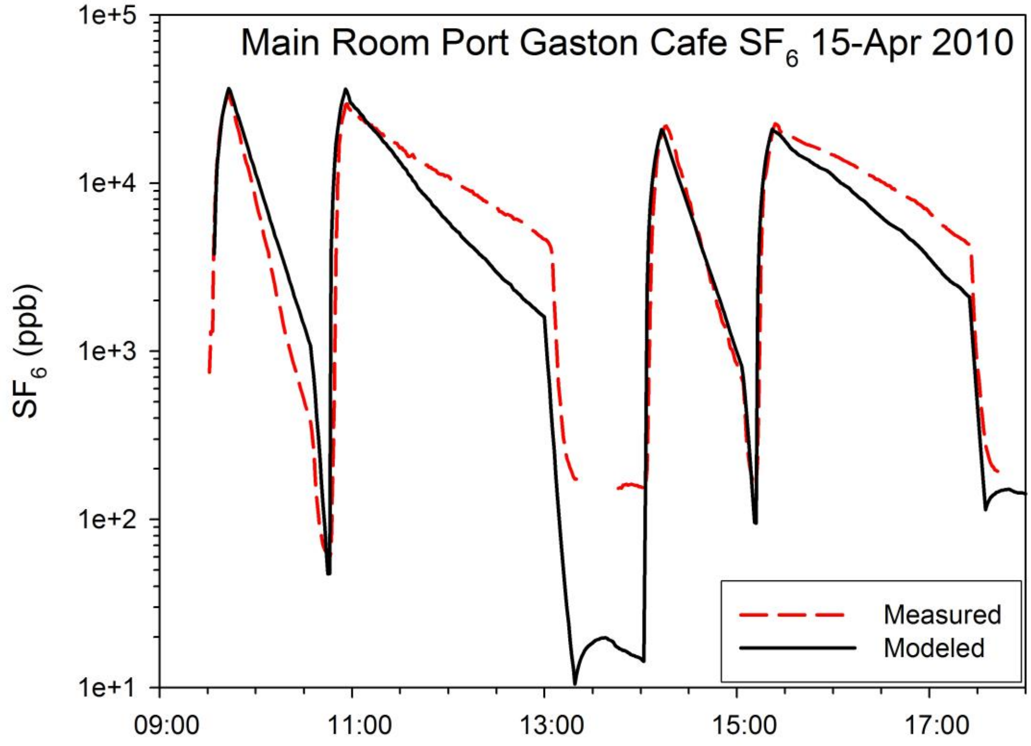


Figure 4.2.1: Model predictions compared to SF_6 measurements in the main room of the Port Gaston building.

4. Work completed for Task 2

4.1 Sampler placement for Hot-Run

The Wet Run/Dry Run (WR/DR) tests showed that the original location of the ground truth instrument manifold #2 (Figure 3.2.1) was exposed to very different TIC concentrations than at locations #1 and #3. Signature Science LLC would like all three manifolds to receive similar concentrations so that all locations reach PEL and IDLH levels equally. They have proposed two alternative sampler placements (Figures 4.1.1 and 4.1.2). Both alternatives move manifold #2 from the lower right room in Figure 3.2.1 to the main room.

LBNL determined that either of the two alternatives would be better than the WR/DR configuration. We concluded this by reviewing the concentration measurements made by the STL Drager Polytron 7000 ECs for each TIC. If the concentrations at various locations in the main room are similar, then we should expect that moving manifold #2 into the main room will bring the concentrations in manifolds #1 and #2 closer.

For example, Figure 4.1.3 shows the concentration measurements of hydrogen chloride at EC sampler locations 1-10 in the main room of the building. At both the PEL and IDLH levels there is good agreement at all locations in the main room; we do not see any local high or low concentrations. We also note that the concentrations at EC 11, which is located in the adjacent room, was somewhat lower the main room. This means that the concentrations in sample manifold location #3 should be watched to ensure that it reaches PEL and IDLH levels.

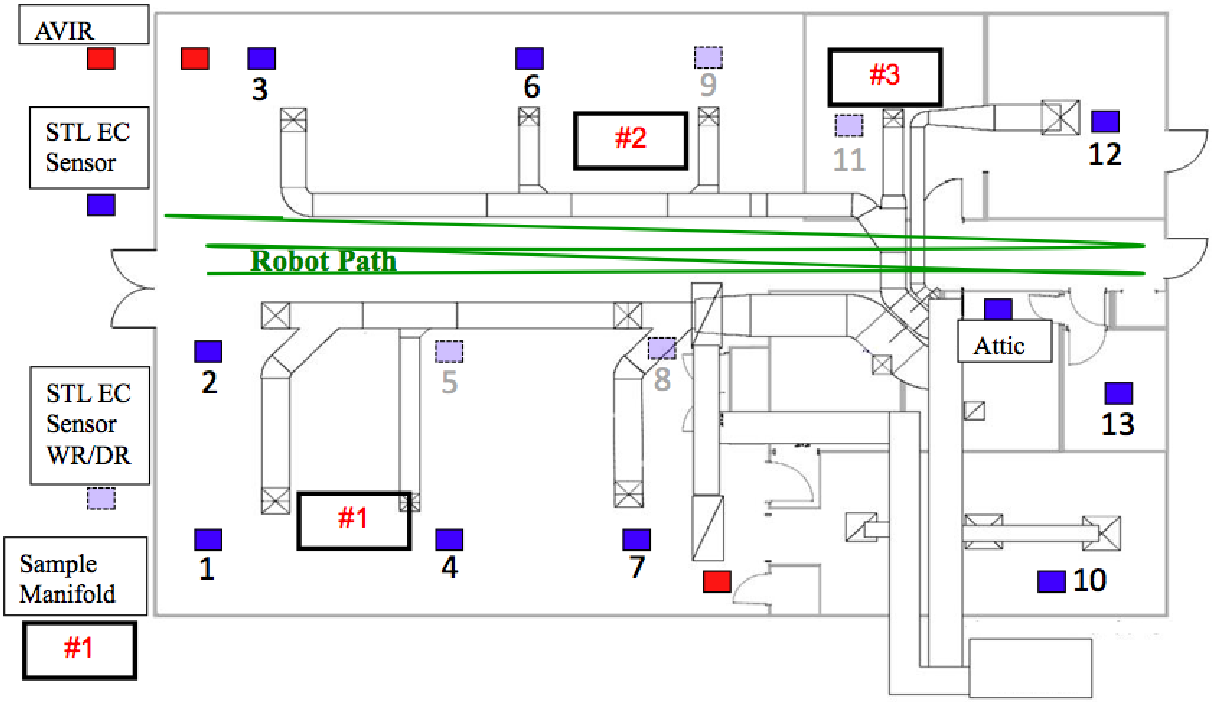


Figure 4.1.1: Alternate #1 location for manifold placement.

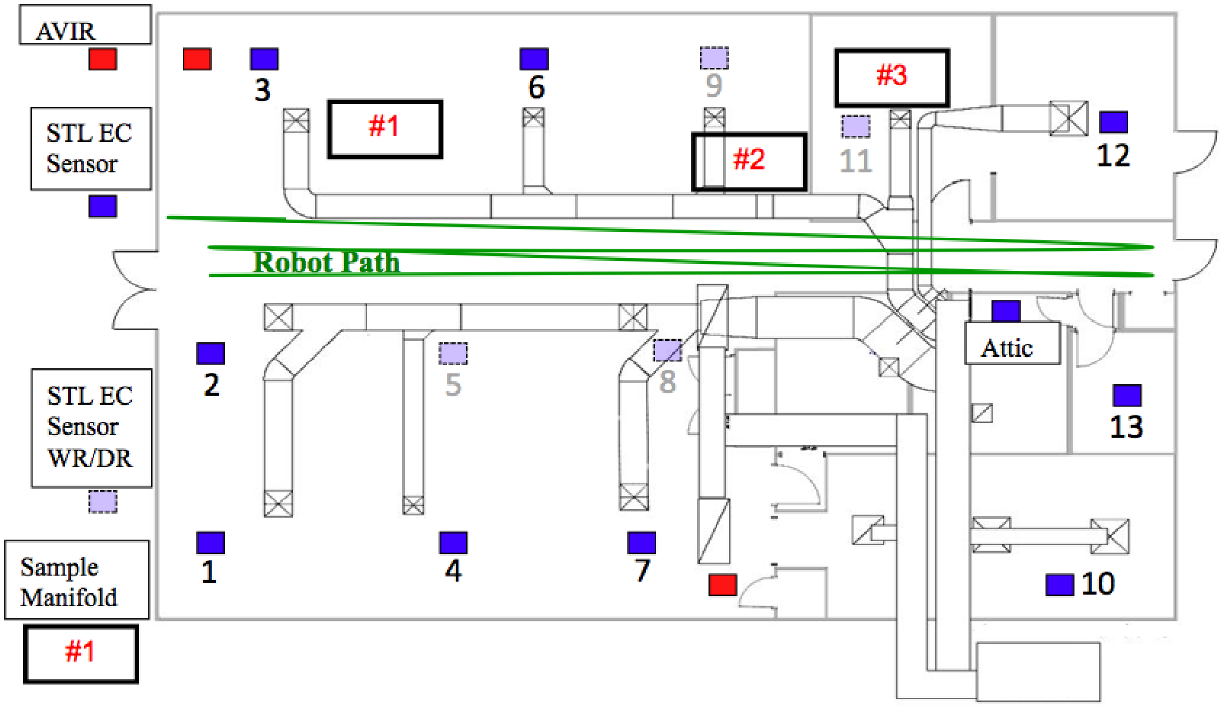


Figure 4.1.2: Alternate #2 location for manifold placement.

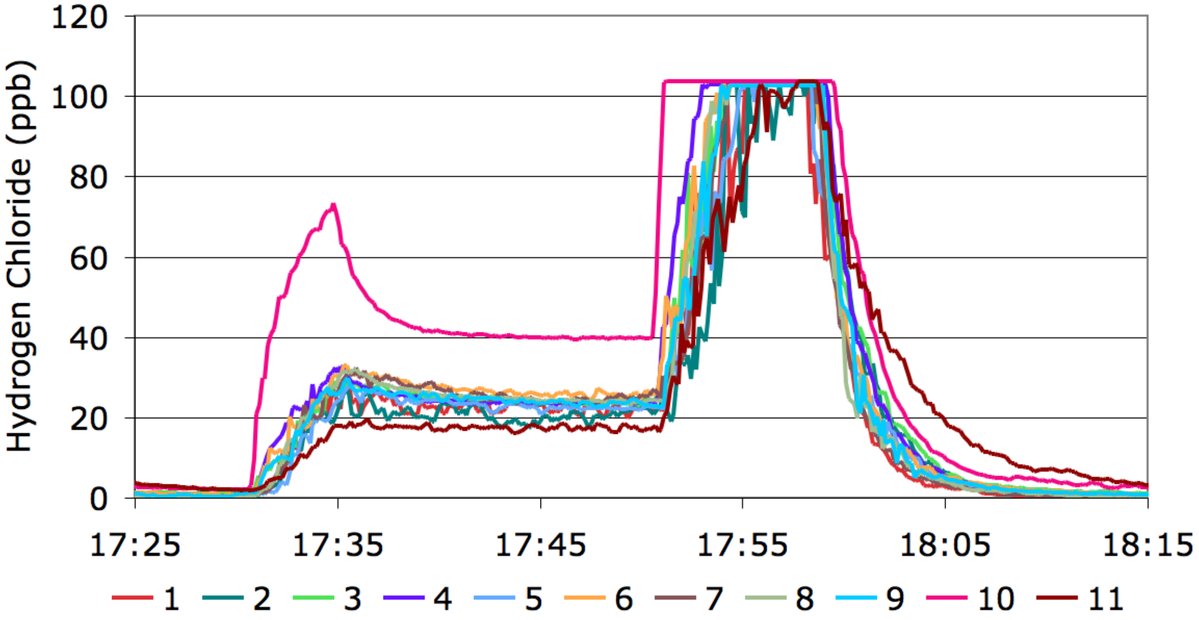


Figure 4.1.3: Hydrogen Chloride concentrations measured at locations 1-11 (see Fig 3.2.1).

4.2 Effect of the meteorological conditions the hot-run test plan.

Signature Science developed a test plan for the Hot Run (HR) based on the results of the Wet Run/Dry Run test (WRDR). The WRDR was conducted in April 2010, and the HR was planned for November 2010. LBNL provided guidance on whether differences in the meteorological conditions, specifically the outdoor wind speed, might affect the setup for the HR.

At high winds, large amounts of fresh air entering the building may mean that more TIC material must be released to reach PEL and IDLH levels. It may also take longer time to reach the said levels. LBNL tested whether the range of wind speeds in November are likely to be so different from the speeds in April that (1) Signature Science must have substantially more TIC material available than planned, based on the WRDR results, or (2) they should be prepared to release at substantially higher or lower rates.

LBNL reviewed historical meteorological records at the Nevada Test Site. Figure 4.2.1 shows the location of the Desert Rock Airport weather station, where 30 years of meteorological conditions were available. Port Gaston is approximately 40 km from the weather station.

First we confirmed that the historical wind readings at Desert Rock Airport could be used as a surrogate for readings at Port Gaston. Figure 4.2.2 shows the range of wind speeds observed at Desert Rock Airport in April, and what was observed at Port Gaston. While not identical, the readings are quite similar. Moreover, the spread in the readings at Port Gaston are quite similar to the spread in readings at Desert Rock.

We next considered the range of wind speeds we expect in November, as estimated at Desert Rock. Figure 4.2.3 show the range of values. The historical records suggest that we see the greatest spread in wind speeds in April, and that November should be less windy. This suggests that the amount of TIC material required for the November experiments will not be significantly different than what was needed for the April trials.

To test whether the rate of TIC release during an experiment might be different in November, we looked at the effect on the indoor concentration for a range of wind speed gusts. Figure 4.2.4 shows the cumulative distribution function of wind speeds expected in November. The median wind speed (CDF=0.5) is approximately 9.25 m/s and the interquartile range (CDF=0.25 to 0.75) is approximately 7.5 – 11.25 m/s. Figure 4.2.5 shows the range of normalized indoor concentrations resulting from a range of wind speeds. To compute the values on the y-axis, we used the CONTAM model to predict the indoor concentration from a steady-state release with the outdoor wind at 7.5 m/s. We then computed the indoor concentration for various average wind speeds (the x-axis) and gusts (the gray area). Finally, we normalized the concentration by dividing the resulting steady-state indoor concentration by the steady-state concentration at 7.5 m/s. The width of the spread at any given wind speed on the x-axis shows how gusts are likely to affect the steady-state indoor concentration. In other words, if the spread was quite wide, then the rate of TIC released during the HR experiments may have to be adjusted quite frequently. The figure shows that the spread is narrow. Even at wind speeds greater than 16 m/s (less than 5% likely to occur from Figure 4.2.4) the spread in the indoor concentration is only about 12%.

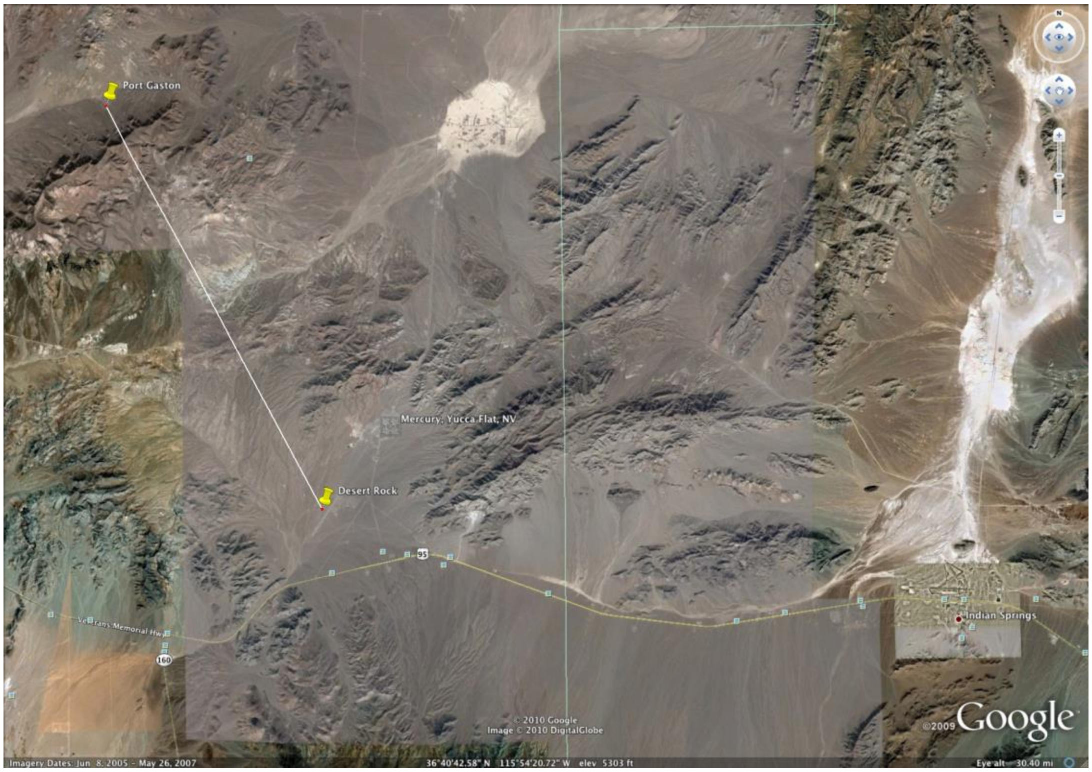


Figure 4:2.1: Locatiosn of Desert Rock weather station and Port Gaston. Port Gaston is approximately 40 km from the weather station.

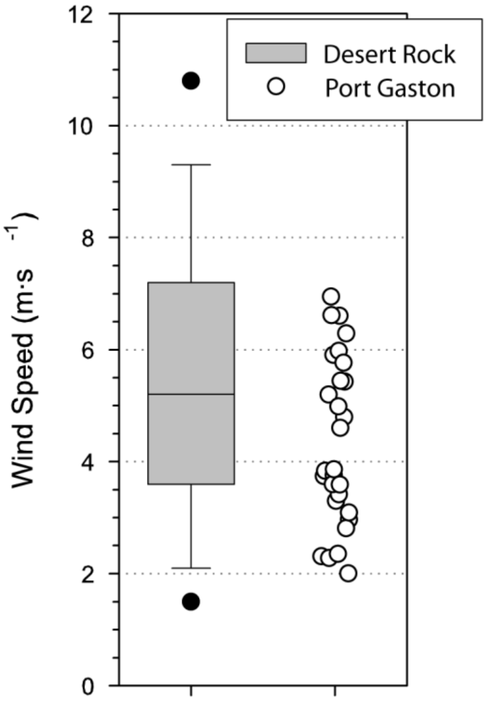


Figure 4.2.2: Comparison of wind speeds observed at the Desert Rock weather station and at Port Gaston in April.

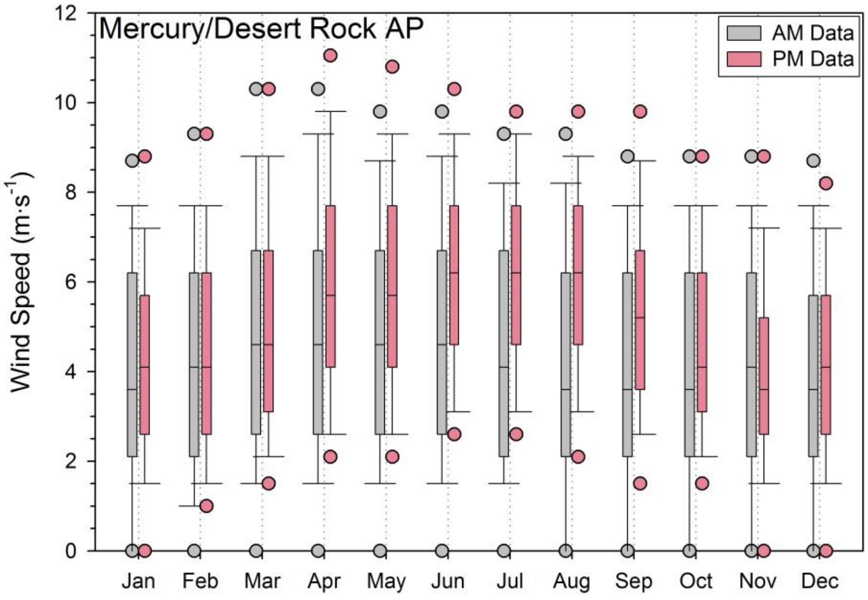


Figure 4.2.3: Thirty years of hourly wind speeds at Desert Rock weather station.

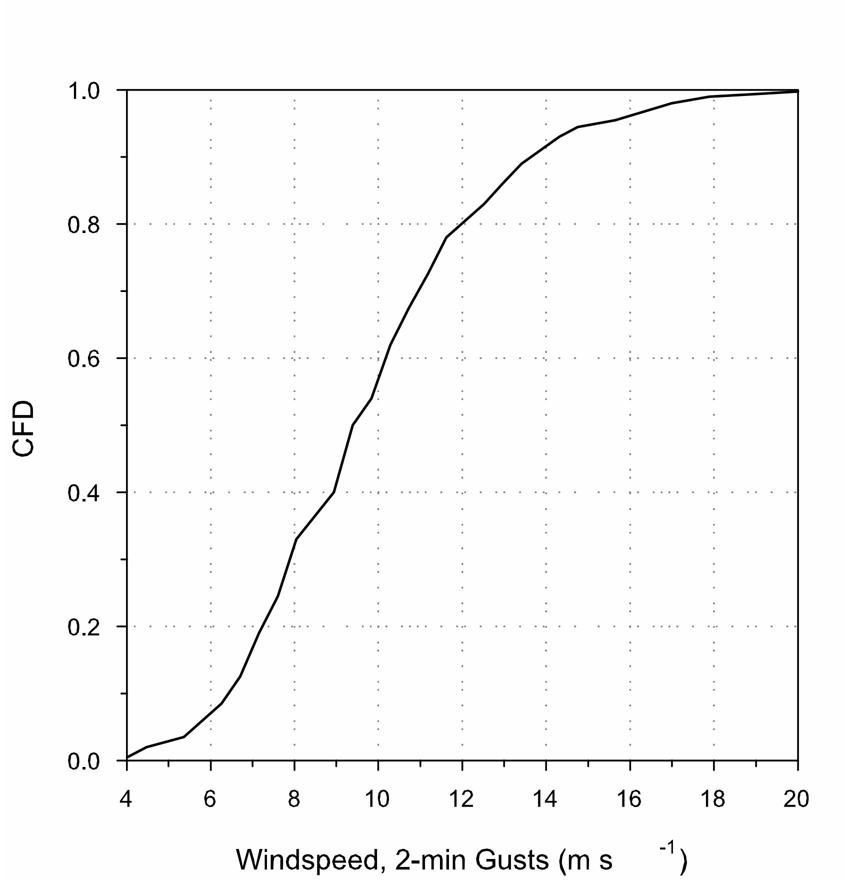


Figure 4.2.4: Cumulative distribution function of 2-min wind gusts at Desert Rock Weather station.

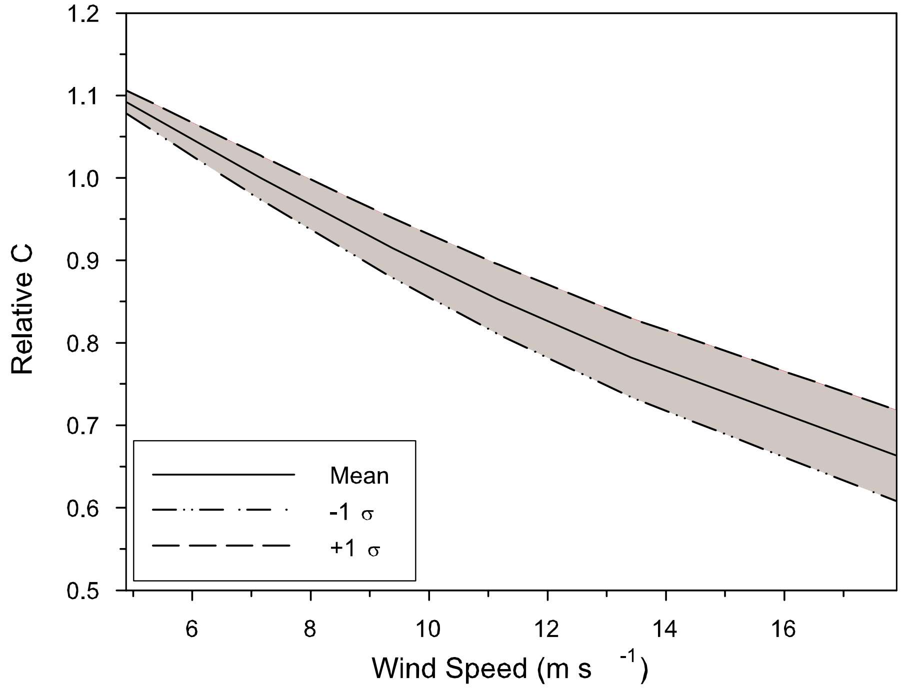


Figure 4.2.5: Normalized indoor concentrations resulting from a range of wind speeds and wind gusts. The value on the y-axis is indoor concentration divided by the indoor concentration at 7.5 m/s.

4.3 Flow in sampling manifold

Signature Science requested guidance on the possibility of "dead spots" in the sample manifold. Argonne National Laboratory and LBNL computed the Reynolds number to be approximately 1040 (flow=110 l/min, viscosity ν=1.58e-4 ft^2/sec, diameter=0.5 ft), which indicates that the flow is laminar. Further, the critical length for fully developed flow is approximately 7 feet (critical length ~ D*4.4*Re^(1/6)). Because the flow through the pipe is neither turbulent nor fully developed, Argonne recommended that air be sampled from within the center of the manifold, rather than from the edge of the pipe, where a laminar boundary layer may be present. LBNL concurs and notes that concentrations of TIC in air is dilute so any dead spots, even if they existed, would not be very different from the bulk air concentration.

5. Experiments to study sorption desorption of toxic industrial compounds

This section presents work that was conducted during the April Wet Run/Dry Run (WD/DR) tests to study if, and to what degree, TICs sorb onto indoor surfaces.

Chemicals in the gas phase have been found to sorb onto indoor surfaces and later desorb (Singer et al., 2004 and Singer et al., 2007). Sorption onto indoor surfaces can lower indoor air concentrations, and can lead to lower exposures to occupants. Desorption on the other hand can lead to a longer duration of compounds in air, and can therefore prolong inhalation exposures. Few studies of sorption/desorption behavior of toxic industrial chemicals (TIC) exist. The Wet Run/Dry Run tests provided a unique opportunity to conduct a scoping study in a real building containing realistic indoor surfaces.

A description of the study is as follows. During the last release on each TIC release day, propylene was released simultaneously with the TIC into the HVAC air intake. The HVAC was turned off and the TIC was measured for 1 to 2 hours. The propylene concentration was measured in each room using a Rae 3000 photo-ionization detector (PID) as shown in Figure 3.2.1. The TIC concentration was measured by Drager Polytron 7000 electro-chemical (EC) detectors, which were operated by NSTSTL. After 1 to 2 hours, the building was ventilated using the auxiliary exhaust fans. Once flushed, the instruments continued to record indoor concentrations overnight to observe possible desorption of TICs from surfaces.

In this study, propylene served as a conservative and inert control gas, meaning it does not sorb to surfaces or react in the gas-phase. We verified that propylene was suitable by comparing indoor decays of propylene with decays of sulfur hexafluoride (SF_6), which is a well-established conservative tracer. SF_6 was measured using Thermo Scientific Miran Sapphire infrared detectors. Figure 5.0.1 shows that propylene and SF_6 decay at nearly the same rates of 1.0 h^{-1} and 0.9 h^{-1}.

Figure 5.0.2 shows the concentrations of propylene and hydrogen chloride (HCl) in the center of the main room. The propylene decays at 1.0 h^{-1}, whereas the HCl concentration decayed at a much greater rate of 3.6 h^{-1}. HCN is sorbing onto indoor surfaces, reacting in the gas-phase, or both.

The decay rates of propylene and HCN at the EC detector locations 1-12 (see Figure 3.2.1) are shown in Figure 5.0.3. Propylene decay rates ranged from 0.7 h^{-1} to 1.8 h^{-1} and hydrogen chloride decay rates range from 2.5 h^{-1} to 3.8 h^{-1}. At each location hydrogen chloride loss is faster than that of propylene. We found similar results for chlorine (Figure 5.0.4).

NH_3 and HCN decayed at the same rate as propylene (Table 5.0.1).

Lastly, no concentrations of TICs were detected overnight. The TIC concentrations were either below equipment detection or it did not desorb off surfaces.

LBNL is reviewing the literature to assess these results, and the implications of them. LBNL will prepare are peer-reviewed journal manuscript of the findings.

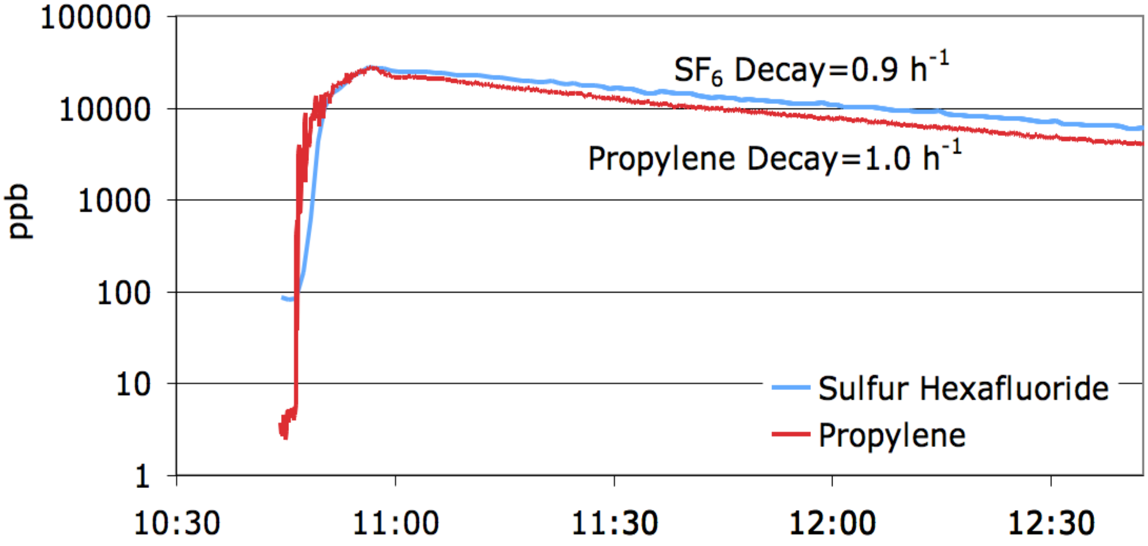


Figure 5.0.1: Simultaneous measurements of SF_6 (blue) and propylene (red) concentrations in the center of the main room.

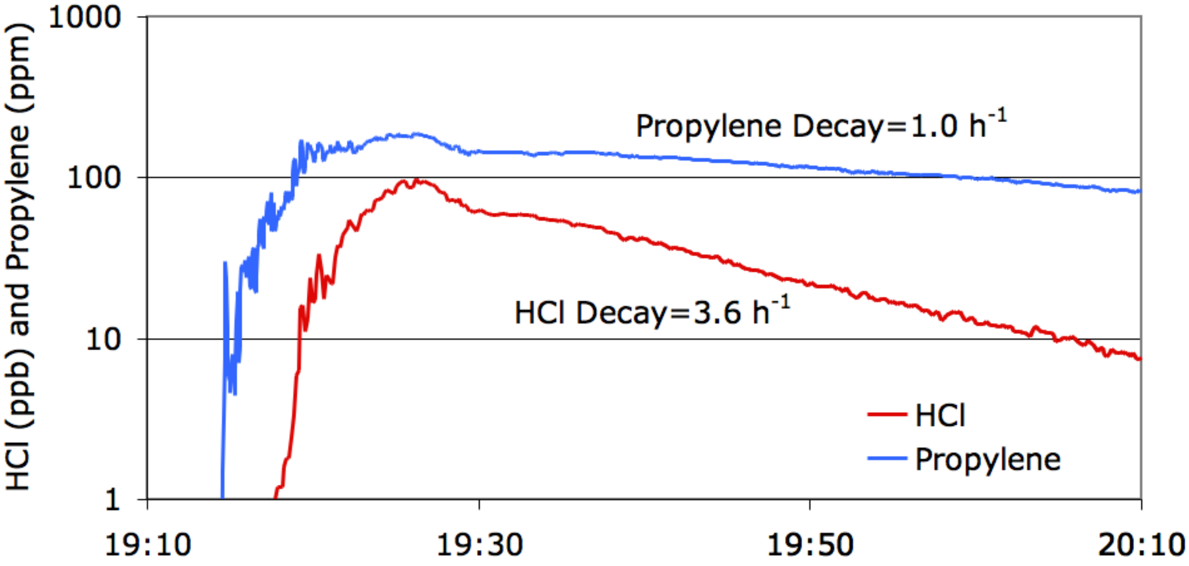


Figure 5.0.2: Simultaneous measurements of hydrogen chloride (HCl, red) and propylene (blue) concentrations in the center of the main room.

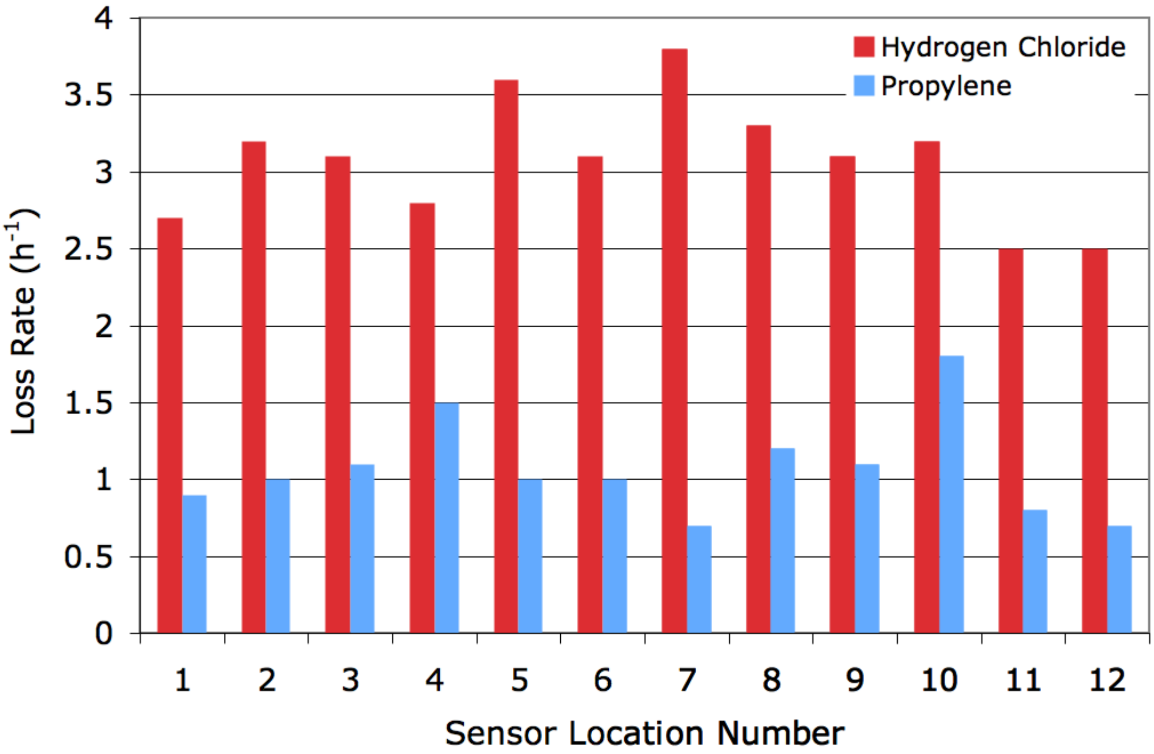


Figure 5.0.3: Loss rates of hydrogen chloride (red) and propylene (blue) at Drager Polytron 7000 locations 1-12 (see Fig 3.2.1).

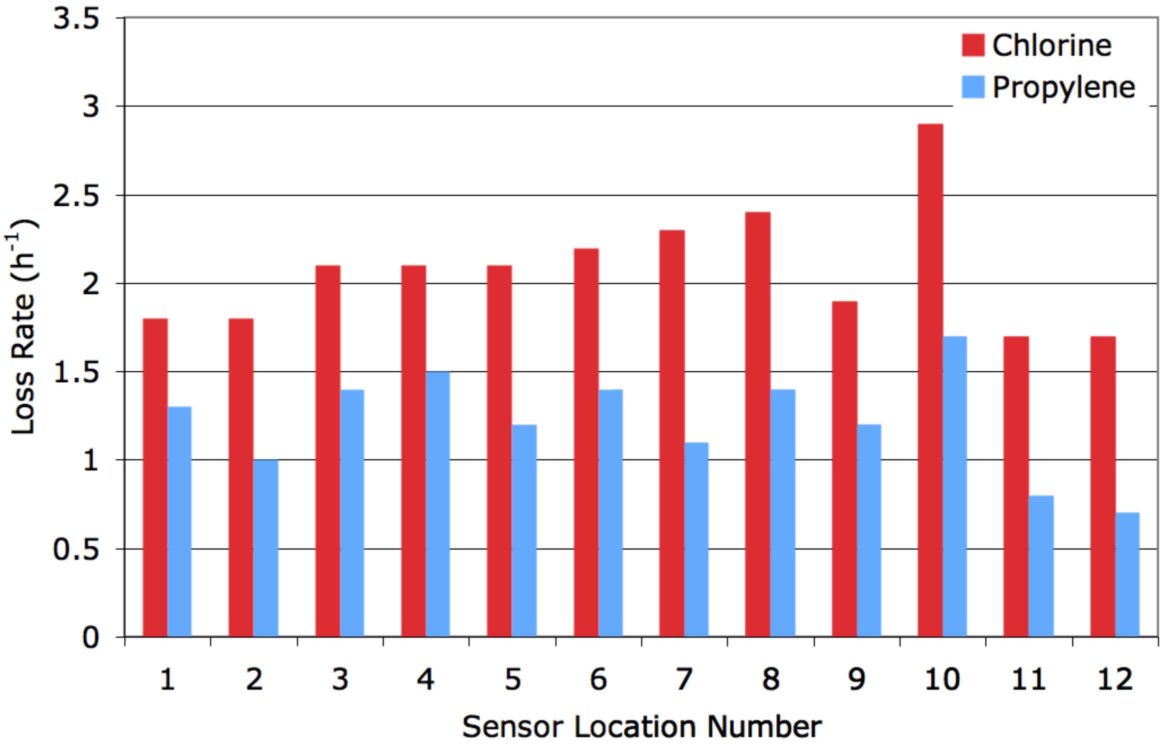


Figure 5.0.4: Loss rates of chlorine (red) and propylene (blue) at Drager Polytron 7000 locations 1-12 (see Fig 3.2.1).

Table 5.0.1: TIC and propylene loss rates and differences between TIC and propylene loss rates averaged over all sensor locations.

	Average Loss Rate (h^{-1})			
TIC	TIC	Propylene	Delta	Notes
HCl	3.1	1.0	2.1	Sorbtion or Reaction
Cl_2	2.1	1.2	0.9	Sorbtion or Reaction
NH_3	2.8	3.2	-0.3	No Sorbtion or Reaction
HCN	1.6	1.7	-0.1	No Sorbtion or Reaction
SO_2	1.5	1.3	0.2	Possible Sorbtion or Rxn

6. Concluding remarks

This document reports on work that Lawrence Berkeley National Laboratory performed to support the Department of Homeland Security's testing of ARFCAM and LACIS systems. LBNL developed a model of the Port Gaston building at the Nevada Test Site and calibrated it using data from field experiments, both blower door and tracer gas tests. The model was developed to (1) support the interpretation of data from field trials performed by Signature Science, (2) support the placement of sampler equipment, and (3) predict if meteorological differences between the Wet-Run/Dry-Run and the Hot-Run might adversely affect the development of the Hot Run Test Plan. In the end, we note that the model was used limitedly because the data from the Wet-Run/Dry Run were if such high quality. LNBL nonetheless provided subject matter support throughout the Wet Run/Dry Run and Hot Run experiments. Lastly, LBNL's experiments of TIC sorb and desorb on indoor surfaces yielded important and new results. The implications of these finding could have important application on DHS-led and -developed sheltering-in-place concepts of operation.

7. References

ASTM E779 - 03 Standard Test Method for Determining Air Leakage Rate by Fan Pressurization. http://www.astm.org/Standards/E779.htm.

Singer B., Revzan K., Hotchi T., Hodgson A., and Brown N., Sorption of organic gases in a furnished room, Atmospheric Environment, 38, 2004, pp. 2483-2494

Singer B., Hodgson A., Hotchi T., Ming K., Sextro R., Wood E., and Brown N., Sorption of organic gases in residential rooms, Atmospheric Environment, 41, 2007, pp. 3251-3265

Appendix A: Experiment test plan

Port Gaston Building 2107 Airflow Characterization Test Plan

Douglas R. Black, Michael D. Sohn, Woody W. Delp
Airflow and Pollutant Transport Group
Indoor Environment Department
Lawrence Berkeley National Laboratory

March 09, 2010 (Version 3)

Table of Contents

1. Overview

The Department of Homeland Security (DHS) plans to test and evaluate prototype chemical detectors developed in the ARFCAM (Autonomous Rapid Facility Chemical Agent Monitor) and LACIS (Lightweight Autonomous Chemical Identification System) Projects in Building 2107 at Port Gaston in Area 26 of the Nevada Test Site (NTS). DHS has selected Signature Science LLC (SSLLC) as the test coordinator and NTS to provide the site building and support. This test plan covers the wet run/dry run tests with ground truth (GT) instruments in three rooms in the building (SSLLC 2010, Fig 2-1). Toxic industrial chemicals (TICs), including ammonia, chlorine, hydrogen chloride, hydrogen cyanide, and sulfur dioxide will be released in the building's HVAC air intake at rates that will result in concentrations that correspond to two alarm levels—permissible exposure limit (PEL) and immediately dangerous to life and health (IDLH). Possible interferents to detection such as floor stripper and diesel exhaust will also be released in the building during the tests.

To support these tests, Lawrence Berkeley National Laboratory (LBNL) will create a CONTAM model of Building 2107 at Port Gaston. CONTAM is a multizone modeling software developed by the National Institute of Standards and Technology (NIST) (http://www.bfrl.nist.gov/IAQanalysis/software/index.htm). The model will be useful for determining the effect of variations in wind speed and direction on the distribution of TIC concentrations in the building and for designing the floor stripper interferent portion of the tests by predicting the floor stripper air concentration that will otherwise not be known because it will not be measured during the tests.

The model will be created from architectural drawings and HVAC specifications provided by NTS. Building leakage parameters are critical to the performance of the model and will be measured by LBNL. The model will be validated using sulfur hexafluoride releases and measurements conducted by LBNL.

LBNL will also design and guide experiments to measure the rate of sorption/desorption of each TIC to/from the building's interior surfaces. While not a requirement to test the prototype detectors, determining the TIC sorption/desorption rates could improve DHS's ability to safeguard against such exposures.

2. Building Characterization Tests and Modeling

2.1 Building Leakage

LBNL will conduct a series of fan pressurization tests to measure the building's leakage characteristics In a fan pressurization test, a high-volume fan blows outdoor air in the building, causing an indoor-outdoor pressure difference. LBNL will measure the pressure difference at various fan flow rates to calculate the effective leakage area in each room of the building. We apply industry methods (ASTM 2009, Sherman 1995) to estimate the leakage area based on the fan flow rate and pressure measurements.

LBNL will also conduct two-fan tests to determine leakage in each room. One fan will drive air from the outside into Room "A", and another will drive air from Room A to Room B. The fans will be placed between doorway thresholds. The differences between flow rates and pressure differences will allow us to map the various airflow leakages throughout the building.

The fan pressurization tests will take one full day and are tentatively scheduled for April 14 (SSLLC 2010, Table 4-2). LBNL will repeat the fan pressurization tests at least twice during the day.

2.2 Tracer Gas Measurements

Sulfur hexafluoride (SF_6), an inert gas tracer, will be released into the building's HVAC air intake (SSLLC 2010, Fig 2-3). SF_6 concentrations will be measured using real-time detectors (Miran SapphIRe by Thermo Scientific) that will be co-located with the ground truth instruments. SF_6 will be released from a gas cylinder through a mass flow controller at a rate of ~20 g/min for ~2 min. The release rates and concentration measurements will be used to calibrate the CONTAM model.

Propylene will be released into the building's HVAC system at a rate of ~20 g/min for ~2 min at the same time as each release of SF_6. Propylene concentrations will be measured with photo-ionization detectors (PIDs; supplied by NTS; six PIDs total) that will be co-located with the SF_6 detectors. Concentrations of each gas will be compared to evaluate the assumption that propylene is an inert tracer.

The SF_6 and propylene tracer experiments will be completed in one day and are tentatively scheduled for April 15 (SSLLC 2010, Table 4-2).

2.3 CONTAM Model

The CONTAM model will be developed and applied for the following purposes:

1. Predict the effect of different wind speeds and direction on concentration distribution in the building;
2. Predict the amount of liquid floor stripper to release in each of the test rooms; and
3. Recommend hardware placements if equal concentrations cannot be met in each of the rooms. This task may be performed by SSLLC by experimentation during the Wet Run / Dry Run tests, but will be later confirmed through modeling to support future experiments.

3. Sorption/Desorption to/from Indoor Surfaces

During the last release on each TIC release day of the wet/dry run, propylene will be released simultaneously with the TIC into the HVAC air intake (SSLLC 2010, Fig. 2-3). The propylene concentrations will be measured in each test room by a PID. Target values for peak propylene concentrations will be 100 ppm, which is far below the lower flammable limit of 24,000 ppm. The decay rates of each TIC, as measured by the ground truth instruments specified and supplied by SSLLC, will be compared to the decay rates of the relatively inert tracer, propylene. Chlorine absorbs to indoor surfaces, while propylene is not expected to so, based on LBNL's research measuring sorption/desorption characteristics of chemicals to/from indoor surfaces (Singer et al., 2004 and Singer et al., 2007). The difference between the decay rates, which can be compared using log-concentration data plots, will provide an estimate of the rate of TIC sorption onto surfaces.

After 1-2 hrs of measuring the decay of the TIC and propylene, the building will be ventilated using the auxiliary exhaust fans. TIC concentrations will be measured and recorded overnight to characterize the desorption rate of the TIC from the indoor surfaces.

4. Health and Safety

The sulfur hexaflouride tracer gas that will be used in this study is a stable, colorless, odorless gas that has been used extensively for outdoor and indoor research, including air-flow and dispersion studies in occupied buildings, for many years in the United States and Europe. It has no known health or environmental effects at the concentrations that will occur during these tests.

Propylene concentrations will be kept well below the lower flammable limit of 2.4% (24,000 ppm). The building will not be occupied during propylene releases.

Material Safety Data Sheets are included in Section 8.

5. Equipment and Supplies

All equipment and supplies will be provided by LBNL except for the six photo-ionization detectors (PIDs) and related datalogging equipment that will be provided by NPTEC, the propylene gas that will be procured by Signature Scientific, and the propylene release mechanism (regulator and flow controller) that will be provided by NPTEC. Two stepladders will also be supplied by NPTEC.

Table 5-1. Equipment and Supplies List

Item	Number	Comments	Packed?
Fan Pressurization Test Equipment (All from LBNL)			
Minneapolis Blower Door—Door frame	4		
Minneapolis Blower Door—Fan and flow rings	4		
Minneapolis Duct Blaster	1		
Automated Performance Test, 8-channel	2		
DG-500 Pressure Gauge	4		
Register shroud for flow measurement	1		
Laptop computer	1		
HOBO Temp/RH sensor and datalogger	6		
Sulfur Hexafluoride Tracer Equipment (All from LBNL)			
Miran SapphIRe	4		
Sulfur Hexafluoride	1	Tracer gas cylinder	
CGA 590 gas cylinder regulator	2		
Mass flow controller	1		
Flow meter	1		
Laptop computer	1		
Gas sample bags	45		
Sample syringes	2	Plastic with leur fittings (no needles)	
2 GB thumb drive	1		
Miscellaneous Equipment (LBNL and NPTEC)			

Table 5-1. Equipment and Supplies List

Item	Number	Comments	Packed?
¼" flexible tubing	300 ft		
Tubing connectors	~20		
Misc toolkit	1	Small, basic kit--screwdrivers, wrenches, etc.	
Flashlight	2		
Masking tape—blue	6 rolls		
Plastic sheeting	1 box		
Sharpie marker	6		
Notebook	2		
Step Ladder	2		NPTEC
Propylene Tracer Equipment (SSLLC and NPTEC)			
Photo-ionization detectors (PIDs)	6	To measure propylene concentrations	NPTEC
Datalogging equipment for recording PIDs	1		NPTEC
Propylene	1	Shipped to NPTEC by SSLLC	
Propylene release mechanism and controller	1		NPTEC

6. Deliverables

LBNL will submit a draft report to DHS one month from the completion of the experiments. Preliminary reports will be available as needed to help plan the final prototype detector tests. The calibrated CONTAM model will be provided to DHS within three months from the completion of these tests.

7. References

SSLLC 2010, *Autonomous Rapid Facility Chemical Agent Monitor (ARFCAM) and Lightweight Autonomous Chemical Identification System (LACIS) In-Facility Tests;* Draft Ground Truth and Chemical Release Field Demonstration and Validation Test Plan (Wet Run/Dry Run Field Test), Rev 2.0

Sherman, M. "The Use of Blower-Door Data," LBNL Report 35173, 1995.

ASTM E1186 - 03(2009) "Standard Practices for Air Leakage Site Detection in Building Envelopes and Air Barrier Systems", ASTM International, 100 Barr Harbor Drive, PO Box C700, West Conshohocken, PA, 19428-2959 USA, 2009, DOI: 10.1520/E1186-03R09 http://www.astm.org/Standards/E1186.htm

Singer B., Revzan K., Hotchi T., Hodgson A., and Brown N., Sorption of organic gases in a furnished room, Atmospheric Environment, 38, 2004, pp. 2483-2494

Singer B., Hodgson A., Hotchi T., Ming K., Sextro R., Wood E., and Brown N., Sorption of organic gases in residential rooms, Atmospheric Environment, 41, 2007, pp. 3251-3265