UCMEXUS FINAL PROJECT REPORT

Collaborative Environmental Chamber and Modeling Studies for Evaluating Effects of Emissions on Air Quality in Mexico City

June 27, 2002

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Executive Summary

Cooperative efforts between the University of California at Riverside through the College of Engineering-Center for Environmental Research and Technology (CE-CERT) and the Mexican Petroleum Institute (IMP) have been carried out. The areas of collaboration were in air quality modeling simulation, environmental chamber experimentation, and chemical reaction mechanisms. During the two-year UCMEXUS project the IMP researchers visited CE-CERT on two separate occasions. Extensive discussions concerning these research areas were held and direct participation on experiments and training courses were undertaken. The bilateral technical effort between IMP and CE-CERT resulted in a number of achievements. Input was obtained on the design of an indoor environmental gas chamber laboratory to conduct reactivity studies of Volatile Organic Compounds (VOC) at IMP. This effort materialized in the construction of a smog chamber facility designed to operate as a Dividable Teflon Chamber (DTC), similar to the gas chambers employed at CE-CERT. The second important area of collaboration focused on air quality modeling using the most recent atmospheric modeling system developed by the USEPA, known as Models-3/CMAQ. New meteorological and air quality data for the Mexico City valley that have become available will be used to conduct collaborative efforts on ozone and aerosol formation with CE-CERT researchers by October of this year. A third important area of interaction concerns the application of the SAPRC-99 chemical mechanism for model evaluation. SAPRC-99 is one of the most advanced explicit photochemical mechanisms developed by CE-CERT that can be used to study VOC reactivity in the airshed. The chamber database from the indoor environmental gas chamber simulations will be used to evaluate the SAPRC-99 chemical mechanism for predicting the effects of VOCs on ozone formation in Mexico City.

Acknowledgements

The investigators want to thank UCMEXUS for the financial support received for this project. We also thank Ms. Irina Malkina, Mr. Kurt Bumiller, and Dr. Claudia Sauer of CE-CERT for helpful discussions about laboratory procedures at CE-CERT and for carrying out the experiments at CE-CERT discussed in this report, Mr. Dennis Fitz at CE-CERT for helpful discussions, and Dr. Zion Wang, Dr. Mohammad Omary and Dr. Bo Wang for valuable assistance and helpful discussions on air quality modeling.

1. INTRODUCTION

In this UCMEXUS final report the cooperative effort between CE-CERT and IMP is presented. The work activities focused on developing the necessary expertise on the airshed modeling area in conjunction with collaboration in the environment chamber area. At the beginning of this project an extended visit of two weeks in September of 2001 was carried out for the purpose of exchanging information and engaging into discussions of the relevance and priorities of the proposed research plan.

In the first extended visit a separate shorter visit to CE-CERT was programmed before the termination of the UCMEXUS project. The second one-week visit took place in mid June of 2002, and the three main tasks to be undertaken were as follows: a) Drafting the report for this project, b) Attending a training session on air quality modeling, and c) participating in some chamber experiments. This second visit included a tour of the facility where the “next generation” environmental chamber is being built to address many of the shortcomings of the existing chamber database (Carter, 2002a), including studies with low NOx concentrations and secondary aerosol formation.

The IMP investigators conducted a compilation and review of existing information concerning captive-air chambers, chamber artifacts, and characterization issues at the initial stages of the collaboration. On the modeling side, the chemical reaction mechanism developed by Dr. Carter (Carter, 2000b) was downloaded into the IMP computers prior to the first IMP visit to CE-CERT. Modeling continues to be a targeted research field for IMP and one of the major purposes of environmental chambers is their utility in testing the portion of the model concerning the chemical reaction and reactivity. Hence acquiring the necessary knowledge at IMP on how to use chamber data for model development and evaluation is essential for determining what experiments would be the most useful and for appropriately interpreting the results of future experiments. The SAPRC-99 chemical mechanism, which is the principal tool for model evaluation is up and running on the IMP computers and computational runs to predict VOC reactivity with SAPRC-99 can be done for the data bases collected from experimentation very soon.

For air quality simulations the latest air quality modeling system available from the USEPA web site, the Models-3/CMAQ (Byun, and Ching, 1999), was also downloaded. The modeling platform for Models-3 was set up in the IMP computers in order to make some air quality simulations (Gipson and Young, 1999) for ozone formation. Further training on the application of this model was received at CE-CERT.

The objectives attained in this project along with a detailed sequence of activities during the time this collaboration lasted are described in the next sections.

2. FIRST *CE-CERT* VISIT

Arrangements were made prior to the IMP visit for participating in some smog chamber experiments. The first visit to CE-CERT took place from September 16 through September 28 of 2001. Two major activities were planned for the first visit, smog chamber experimentation and modeling work.

2.1 Gas Chamber Experiments

The experiments were carried out using an Indoor Teflon Chamber that was employed in previous chamber characterization studies by CE-CERT (Carter, 2002a). It consists of a ~3000-liter Teflon film "pillowbag" reactor with a blacklight source. The Teflon film reaction bag was located inside a larger Teflon film bag continuously flushed with purified air, which in turn was inside an enclosure fitted with the light source. The light source consisted of two opposed walls holding banks of Sylvania 40-W BL blacklights. Dry purified air was provided by an AADCO air purification system, with further purification accomplished using Hopcolite.

The chamber was flushed with dry purified air on the night before the experiment. Then the measuring analyzers for ozone and NOx were connected to a logging data acquisition system. The preparation of the feed into the reactor was shown and the procedure for injecting the VOC-NOx mixture was observed. The mixture

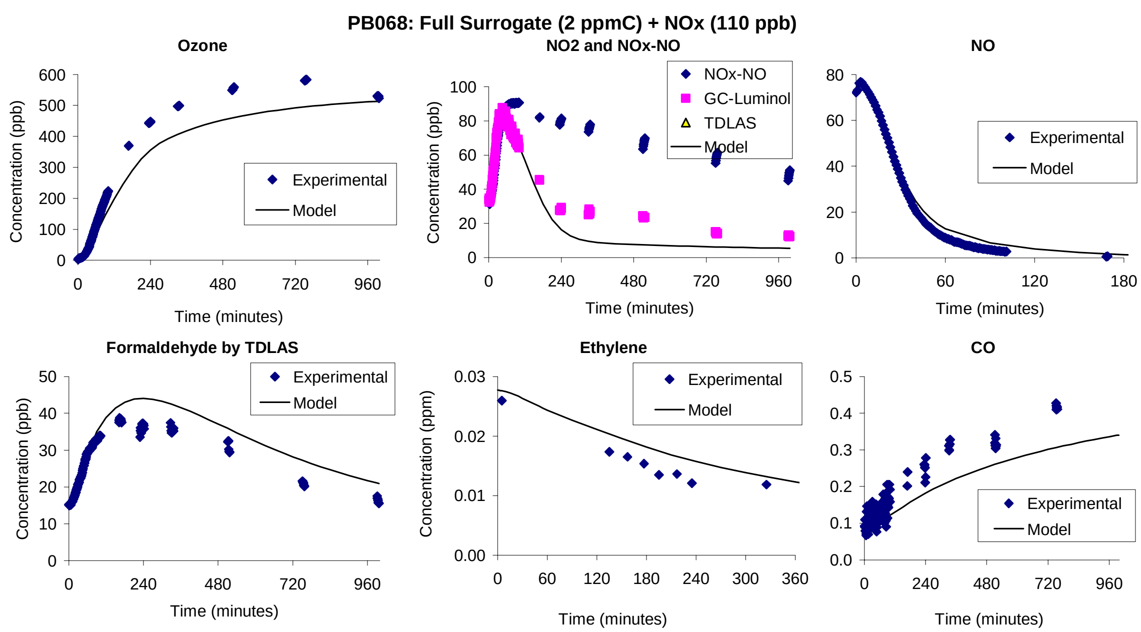

Figure 1. Selected experimental and model calculation results of the photochemical smog simulation experiment carried out at CE-CERT for the IMP collaborators

fed into the smog chamber consisted of VOCs and NOx. The reactants were mixed by manual agitation of the reaction bag. Later on the black light source was turned on and the progress of ozone production was recorded. Ozone and NOx were monitored and the output from the measuring instruments, along with that from temperature and light sensors were attached to a computer data acquisition system, which recorded the data at periodical intervals. Gas Chromatography (CG) measured organic reactants. The samples were taken from ports directly connected to the chamber. More details concerning the experiment are described by Carter (2002).

Examples of data obtained during the experiment are shown in Figure 1, along with results of model simulations of the experiment using the SAPRC-99 mechanism. This mechanism and the software to simulate the experimental results and recommended input data for modeling such experiments were provided to the IMP researchers during their first visit.

The first visit also focused on some of the most important aspects of airshed modeling. Air quality modeling work was performed at CE-CERT in order to gain more experience on the preparation of input files to drive air quality models. Of particular interest was the modular structure of Models-3/CAMQ under the UNIX platform. One of the problems that IMP research group had been having before coming down to CE-CERT was getting the script files of Models-3 to work. A working session was devoted to resolve this problem so that the Ozone base case embedded in the stand-alone version of CMAQ could be run at IMP. Another modeling activity centered on the emission processing system of SMOKE, which is one of the modules of Models-3 that deals with the emission inventory. The tree diagram of the various script files and input data files that are needed by SMOKE were reviewed, and the graphical interface to visualize the modeling results with PAVE were examined in great detail. The material covered during these discussions gave researchers at IMP a familiarity with the experience at CE-CERT concerning the latest air quality computational tools for model simulation of surface ozone formation.

2.2 The New Environmental Gas Chamber Laboratory at IMP

After the first two-week visit to CE-CERT some progress has been attained during the last months in regard to the objectives stated in the collaborative proposal submitted to UCMEXUS. The advancement centers primarily on the construction of a new gas chamber facility at IMP initiated in August of 2001. The design was based following the CE-CERT guidelines described by Dr. Carter and his group during the two-week visit last September.

The new environmental gas chamber laboratory was planned for completion in two phases. The research team at IMP plans to carry out both indoor and outdoor smog chamber experiments starting by the end of this year. The first phase of the project, which concerned all labor for the indoor chamber facility to conduct VOC reactivity studies, has been completed. This included the layout of the laboratory adhering to safety procedures, and the purchasing of analytical equipment needed for measuring ozone and its precursors. The facility is located on the roof of a two-story IMP building.

Enough room has been allowed to house a Dividable Teflon Chamber (DTC), including instrumentation and the analytical equipment that integrates the new facility. The second phase of the smog reactor facility has to do with the construction of the DTC itself. This last phase that is still underway is expected to be completed by December of 2002. Although the new indoor smog chamber is being built based on DTC-CECERT design, new adaptations have been added to the original design to make it more suitable for investigating temperature variations on VOC reactivity-studies for the air shed of Mexico City.

The new DTC design (see Appendix) is similar to the design of the CE-CERT DTC as described by Carter et al (1995). The IMP chamber contains two 5000-liter reaction bags placed adjacent to each other. It features an air conditioning system that controls room temperature variations ranging from 15 C to 35 C. By controlling the outside air temperature the effect of temperature on reactivity of VOC's can be better studied. An AADCO air purification system located next to the indoor chamber will supply pure dry air. A dryer will be adapted to the AADCO purification system to further improve its efficiency.

In the same facility a laboratory bench area is reserved for both analysis of collected samples with commercially available continuous analyzers and the computer data acquisition system, which will record the monitored data. This area will also be used for the preparations of mixtures fed into the Teflon reaction bags. Three chromatographs (GC-SM, a GC-ECD and a GC-FID HP 6890), each one with different detectors complements the laboratory, and for spectral measurements, a LiCor Li-800 portable spectroradiometer has been acquired. For measuring ozone there is a UV photometry-ozone analyzer Teco model 49C, while the nitrogen oxides and total oxides of nitrogen are analyzed using a chemiluminescent NO Teco model 42C. The output of these instruments along with that from the temperature and light sensors are going to be fed to a computer data acquisition system ESC model 8816. Up till now different methodologies are being tested to measure VOC, aldehydes, ketones and PANs. When the IMP indoor chamber facility is completed, experiments of mutual interest between CE-CERT and IMP could be carried out to deepen more into the complex atmospheric chemistry, particularly that of the Mexico City Basin or Los Angeles.

2.3 Field Study in the Mexico City Basin

As part of the activities that are linked to the gas chamber experimentation and air quality modeling, a field study for hydrocarbon and meteorology measurements was carried out in the Mexico City Metropolitan Area (MCMA) for six days (April 30, May 3, May 5-7, and May 14) in May of 2002. There are two main reasons for taking on this new field study. Firstly, fresh meteorological and air quality data are needed to test the predictability of both meteorological and photochemical transport and dispersion models. Secondly, with the new IMP indoor gas chamber facility a representative VOC profile for the MCMA is required to conduct VOC reactivity studies that are needed for implementing air quality control strategies.

The air quality campaign focused on measuring hydrocarbons, chlorinated compounds, and carbonyls including both aldehydes and ketones. This air quality study was decided based upon historic episodes of high ozone production in the Mexico City Basin. Concurrently, three meteorological balloons were launched simultaneously with a radio sounding system at several times throughout the days that the field study lasted using DIGICORAS III. Surface meteorological data was also gathered at the same locations where the soundings were released. This database will be used for modeling work between CE-CERT and IMP.

2.4 Air Quality Modeling at IMP

Since the beginning of the UCMEXUS jointly effort the IMP modeling group has been active and working on setting up the meteorological model MM5 and the transport and conversion code for CMAQ that will be used for studies on ozone formation in the Mexico City basin. This modeling pair conforms the Models-3 system. The output from these two computer models will be evaluated by comparing predicted results with collected data obtained during the field study of last May. The Mesoscale Modeling System, MM5, which is responsible for calculating the three-dimensional wind fields and temperature fields that drive the photochemical model, CMAQ, is now running with topography and geophysical data for the Mexico City Metropolitan Area.

After receiving training from the CE-CERT experts on modeling last September, simulations were performed at IMP in a workstation SGI for the database that comes with the CMAQ modeling package. The database is for modeling the July 14, 1995 episode on ozone of Eastern US. The photochemical mechanism that was used to describe the atmospheric chemistry was the Carbon Bond IV (Adelman, Z.E., 1999). The spatial horizontal resolution for this run was 36 kilometers, and the domain of interest encompasses a big portion of the US as shown in Figure 2. Figure 2 shows the geographical location of the modeling domain and the fraction of urban land use distribution within the region.

Figure 3 depicts surface ozone distributions in ppm at two times for the simulated period. Figure 2 and Figure 3 were produced using the visual interface PAVE, which is a module of the modeling systems, Models-3.

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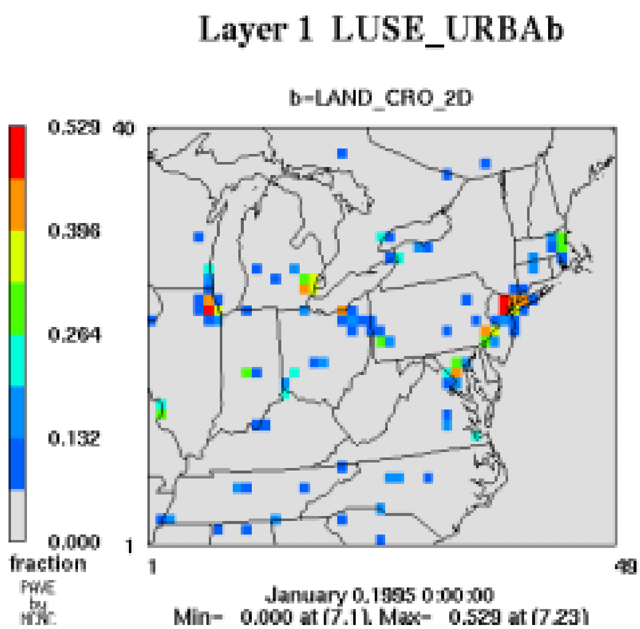

Figure 2. Map showing the fraction of urban areas (base case).

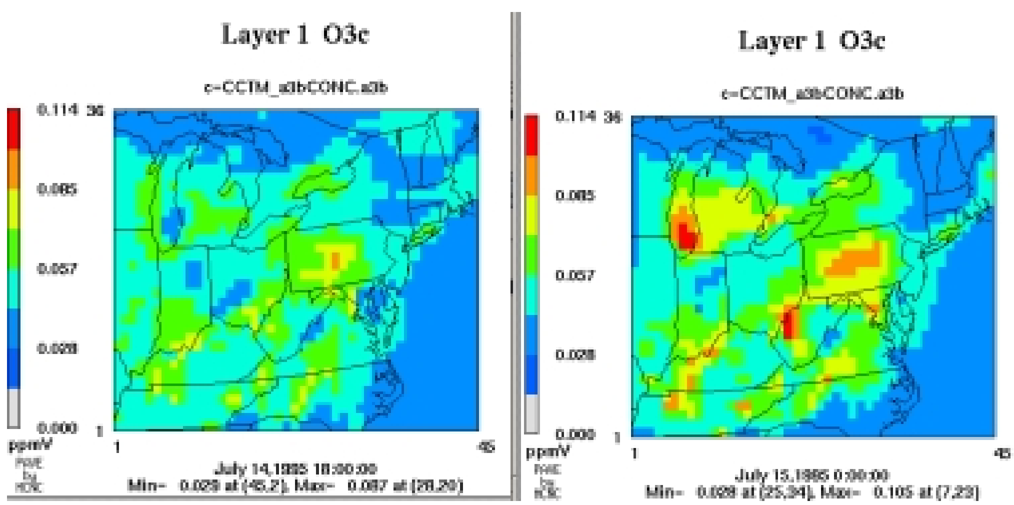

Figure 3. Surface ozone concentrations of the simulated run on Eastern US.

3. SECOND *CE-CERT* VISIT

The second visit took place from June 10 through June 13, 2002. In this visit the IMP group participated in several chamber experiments to study VOC reactivity (Carter, 1994), received further training on the photochemical model, CMAQ, and the emission processing system, SMOKE. The CMAQ and SMOKE modules are part of the Models-3 system, which the IMP team will use for air quality simulations in the Mexico City Metropolitan Area. Part of the time in the second visit was devoted to the preparation of the final report.

3.1 Gas Chamber Experiments

The experiments were performed in the new CE-CERT facility that will house a new state of the science environmental gas chamber that is currently under construction (Carter, 2002a). Three smog chamber experiments were carried out in a Small Teflon Chamber (STC) that was recently built at CE-CERT. The STC was used because construction of the new, much larger CE-CERT chamber is not yet complete. This chamber consists of a 4’ x 4’ x 8’ enclosure with a single Teflon bag reactor. The enclosure was designed with two panels of blacklights evenly distributed on the top and bottom of the enclosure totaling 64 light bulbs. The ~4000-liter Teflon film was injected with a VOC mixture and amounts of NO and NO_2 concentrations. The initial concentrations for the STC surrogate experiment (all in ppm) are as follows. Propene (0.012), Toluene (0.025), M-Xylene (0.016), Formaldehyde (0.061), Propane (0.166), n-Butane (0.075), and Acetaldehyde (0.029). This was designed by the IMP researchers to be a highly simplified surrogate of Reactive VOC pollution in Mexico City.

This surrogate mixture was taken as the base case. Acetaldehyde was initially considered in the surrogate composition but after performing a model evaluation it was found that this compound did not make much of a difference in the calculated ozone levels or most other species, except for PAN. Because its presence in the surrogate mixture complicated the experimental procedures and analysis, it was removed from the surrogate mixture to make the experiment simpler. Single preliminary modeling was done to specify the NOx concentration that would yield a peak ozone concentration within five hours of irradiation, which was considered to be most useful for the base case. The modeling results yielded a concentration of 0.05 ppm of NO_x, which was apportioned to 0.05 ppm of NO, and 0.01 ppm of NO_2.

A standard operating procedure and data processing was followed for every run. The reactor was emptied and then refill with air, repeating this procedure several times. The bag was left with dry pure air the night before the experiment. Next day the bag was emptied and filled with fresh pure air. Then background concentrations were checked and samples were taken for GC. It was verified that all analyzers (CO, NOx, PAN, O_3) were working properly. Surrogate mixture was prepared using a vacuum rack. The reactants were injected into the reaction bag, introducing first the $NO-NO_2$ mixture, followed by the VOC reactants. Liquid VOC such as Toluene and M-Xylene were injected through a heated tube. Enough time was allowed for the reactants to mix while the bag was manually agitated to enhance mixing. Sampling lines were connected to analyzers to monitor the evolution of the reaction. Mixing was assumed to be complete when the response of every analyzer became stable. Before the blacklight source was turned on a gas sample was drawn for GC to verify if target initial VOC concentration was correct. Samples were taken from the bag at regular time intervals to monitor the evolution of the photochemical reaction inside the reactor. Automated program was started to sample every 45 minutes for a 15-minute period. When the experiment ended the bag was flushed and the procedure repeated for the next experiment.

The experiments that were carried out for this project in conjunction with the second IMP visit are summarized on Table 1. As indicated there, reactivity experiments were performed for two species, involving a base case experiment and separate runs with added Propane or m-Xylene. An additional experiment was carried out with the toluene and m-xylene concentrations higher than intended for the base case, so this served as an additional experiment on the effects of aromatics. The results of the experiments are summarized on Table 1, and representative concentration-time plots for O_3 are shown on Figure 4 and Figure 5.

Complete analysis of the results of the experiments will be carried out primarily at IMP after the conclusion of the program, and will be used to familiarize them with modeling and analyzing indoor chamber reactivity experiments for model evaluation. Preliminary modeling of the experiments, using the SAPRC-99 mechanism, was carried out at CE-CERT, with the results for O_3 shown on Figure 4 and Figure 5. The files with the experimental data and model input were transmitted to IMP for their analysis.

3.3 Training Course in Air Quality Modeling

During this second visit one of the IMP visitors attended the Western Regional Air Partnership training course lectured by Dr. Gail Tonnesen. The core of the presentation focused on the USEPA Community Multiscale Air Quality Model, CMAQ, and emission processing procedures described by the Sparse Matrix Operator Kernel Emissions Modeling System, known as SMOKE.

The training course lasted for five days and had as the main target to expose the attendant to perform air quality modeling using the Community Multiscale Air Quality, Models-3/CMAQ. The training course initiated with an introduction to basic principles on Air Quality Computational Simulation. The course focused on the operational aspects of the photochemical model development work under the Models-3 environment. A general analysis of the CMAQ source code structure, and the CMAQ execution environment in Models-3 was presented. Concepts used in the study of transport, transformation and dispersion of atmospheric pollutants were defined. Then the UNIX operating system was introduced and basic commands were reviewed to aid the modeler in navigating into the computer

Table 1. Summary of CE-CERT environmental chamber experiments carried out during the second IMP visit in June

Run	Description	Experiment	Results and Discussion
STC-001	NO2 Actinometry	No reactor in the chamber. NO_2 photolysis rate measured using quartz tube method (Carter et al, 1995). Carried out prior to IMP visit for light characterization.	NO_2 photolysis rate without the reactor was 0.77 min-1.
STC-002	Pure Air	Purified air irradiated for 7.5 hours. Carried out prior to IMP visit for characterization purposes.	25 ppb of O_3 formed after ~25 hours. Data base fit by model assuming NOx offgasing rate of ~0.2 ppb/hour. Results as expected for this type of reactor.
STC-003	CO - Air	0.2 ppm NO, 0.08 ppm NO_2, and 78 ppm CO injected and irradiated for 5.5 hours. Carried out prior to IMP visit to characterize the chamber radical source (see Carter et al, 1995).	~0.18 ppm O_3 formed in about 5.5 hours. Data best fit by model assuming a radical input rate of ~35 ppb/min. This is high for this type of reactor, but may be due to the relatively high temperatures in these experiments, which were in the range of 310-315^o K.
STC-004	Surrogate - NOx with high aromatics.	Intended to be experiment with standard base case surrogate concentrations (see text), but toluene and m-xylene injections were ~10 times higher than intended. ~5 hour irradiation.	Results similar to the added m-xylene run STC-006. Initial O_3 formation rate very rapid, with ~0.2 ppm being formed in the first 20 minutes. Peak O_3 concentration was ~0.28 ppm after about 8-hours of irradiation.
STC-005	Base Case Surrogate - NOx	Base case surrogate experiment using surrogate and NOx levels discussed in the text. ~5 hour irradiation.	~0.2 ppm O_3 formed in the first hour. O_3 was ~0.44 ppm after 5 hours, and still increasing slowly. Experimental and calculated O_3 data are shown on Figure 4 and Figure 5, where they are compared with the experiments with added propane or m-xylene.
STC-006	Surrogate - NOx + propane	Same reactants as STC-005 except initial propane increased to 7.8 ppm.	Ozone formation rate and peak O_3 was higher than base case experiment, with ~ 0.3 ppm being formed in the first hour, and 0.67 being formed at 5 hours. The results are shown on Figure 4, where they are compared with the results of the base case experiment.
STC-007	Surrogate - NOx + m-Xylene	Same reactants as STC-005 except initial m-xylene increased to 0.2 ppm.	Results similar to STC-004 except final O_3 was somewhat higher. About 0.2 ppm O_3 formed in the first 20 minutes, and the peak O_3 of ~0.3 ppm occurred after about 3 hours of irradiation, then it declined slightly after that. The results are shown on Figure 5, where they are compared with the results of the base case experiment.

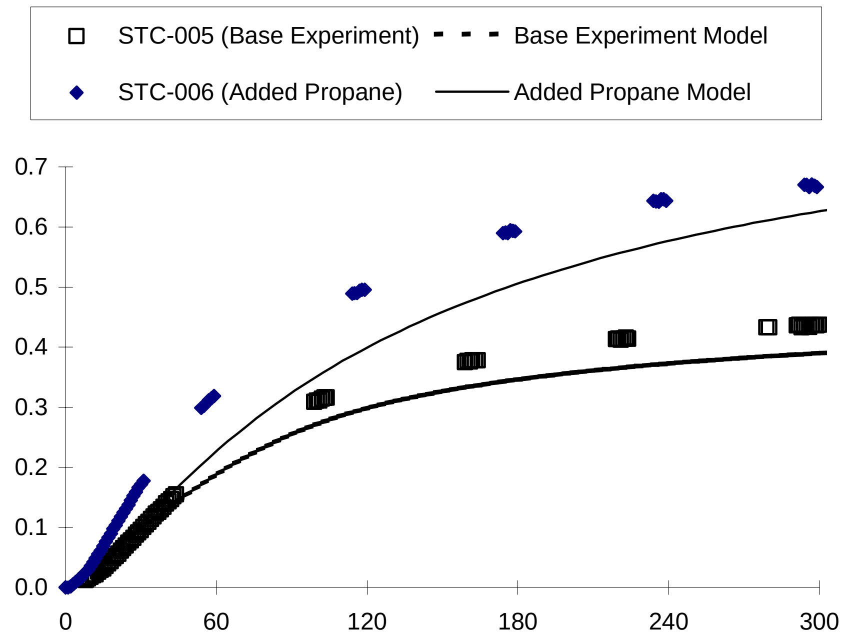

Figure 4. Experimental and calculated concentration-time plots for the base case and the added propane surrogate-NO_x experiments

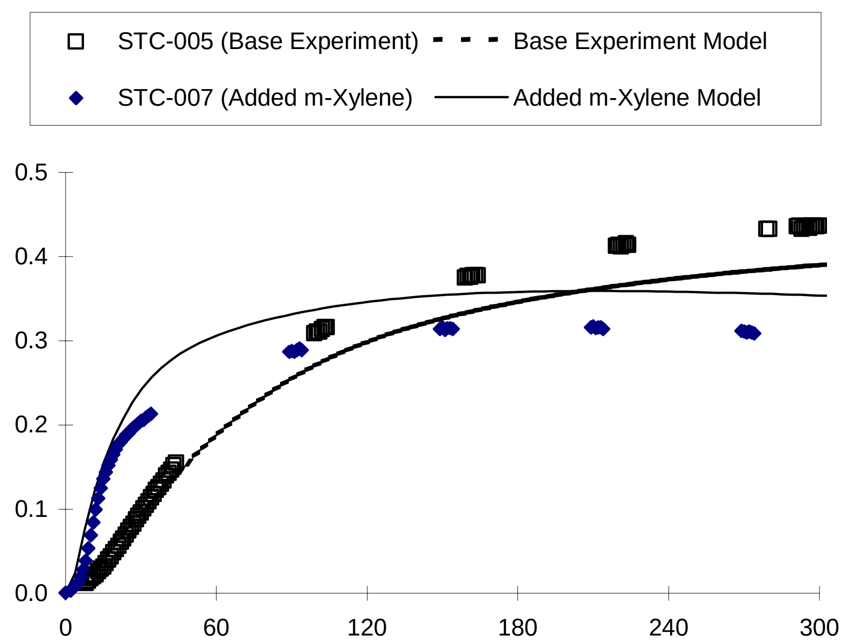

Figure 5. Experimental and calculated concentration-time plots for the base case and the added m-xylene surrogate-NO_x experiments.

platform under which files can be managed, and programs compiled, linked and executed. The utility program CVS (Concurrent Version Control System) was discussed in order to learn how to manage the creation of script files (Makefile) for managing simulation runs, including the utility I/O API (Input/Output Applications Programming Interface). A description of how to use the Package for Analysis and Visualization of Environmental data, called PAVE, was given. PAVE is a flexible application to visualize multivariate gridded environmental data

Several important modules embedded in CMAQ were explained in detail. These included the following modules: a) Initial conditions (ICON), b) Boundary conditions (BCON), c) Photolysis rates (JPROC), d) Meteorological preprocessor (MCIP), e) Introduction to Gas phase chemistry, f) Chemical transport model, g) Process analysis (PACP), h) Aerosol dynamics and chemistry, and I) Model evaluation.

The training session was a hands-on approach, so the attendant had the opportunity to verify what the training team had taught, and to reproduce modeling results for better understanding of the application of CMAQ. As a practical application of regional air quality modeling, the REMSAD (Regulatory Modeling System for Aerosols and Deposition) was run.

The last segment of the course consisted on a discussion of the procedures to handle the emission processing system through the SMOKE computer code, which allows emissions data processing methods to integrate high-performance-computing (Houyoux, 2000). The advantage of using the SMOKE system for decision making about emissions controls for both urban and regional applications was discussed. The main use of SMOKE for providing a mechanism for preparing specialized inputs for air quality modeling research was one of the objectives of this lecture.

3.3 The SAPRC-99 Chemical Mechanism

Sensitivity tests will be done on SAPRC-99 introducing constants calculated by the “ab initio” values obtained in IMP using the molecular simulator Gaussian98. This phase will aid in adjusting some of the mechanistic parameters in SAPRC-99 of a few typical VOC explicit chemical reactions that take place in Mexico City airshed. In this regard we have been looking into Tables A-2 to A-4 (of the Carter, 2000b) to find out the reactions where the “ab initio” values obtained through calculations at the IMP could be appended to SAPRC-99. The next most important application of SAPPC-99 is for the indoor environmental gas chamber simulations which will be used to evaluate the ability of the mechanism to simulate the effect of VOCs on ozone formation in Mexico City.

4.CONCLUSIONS

The objectives of the cooperative effort between CE-CERT and IMP have been successfully accomplished. This precedent-setting approach of this collaboration has sought a permanent linkage to enable its participants as leaders in the field of air quality research, and to create a long-term collaboration for future project.

New meteorological and air quality data for the Mexico City valley that are now available will be used to conduct collaborative efforts on air quality simulations with CE-CERT by October of this year. In this line of work an inter-comparison between Models-3/CMAQ and other regulatory air quality models can be performed to shed new light in the skills of each model and their limitations.

When the IMP indoor chamber facility is completed this year experiments to be performed will be designed to measure the incremental reactivity of various organic species when added to surrogate VOC-NOx-Air mixtures representing the urban Mexico City atmosphere. Computer modeling of environmental chamber measurements of incremental reactivity of VOC will be pursued in order to evaluate a detailed atmospheric photochemical mechanism for airshed models that predict ozone in Mexico City.

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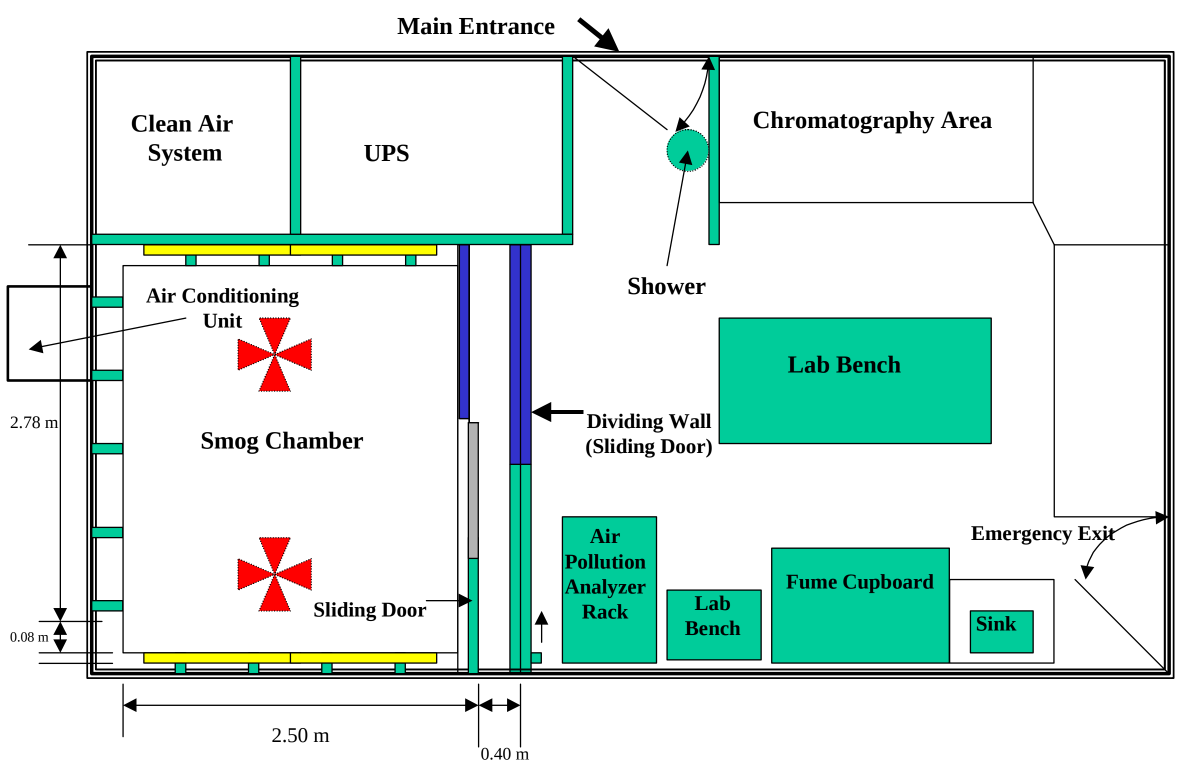
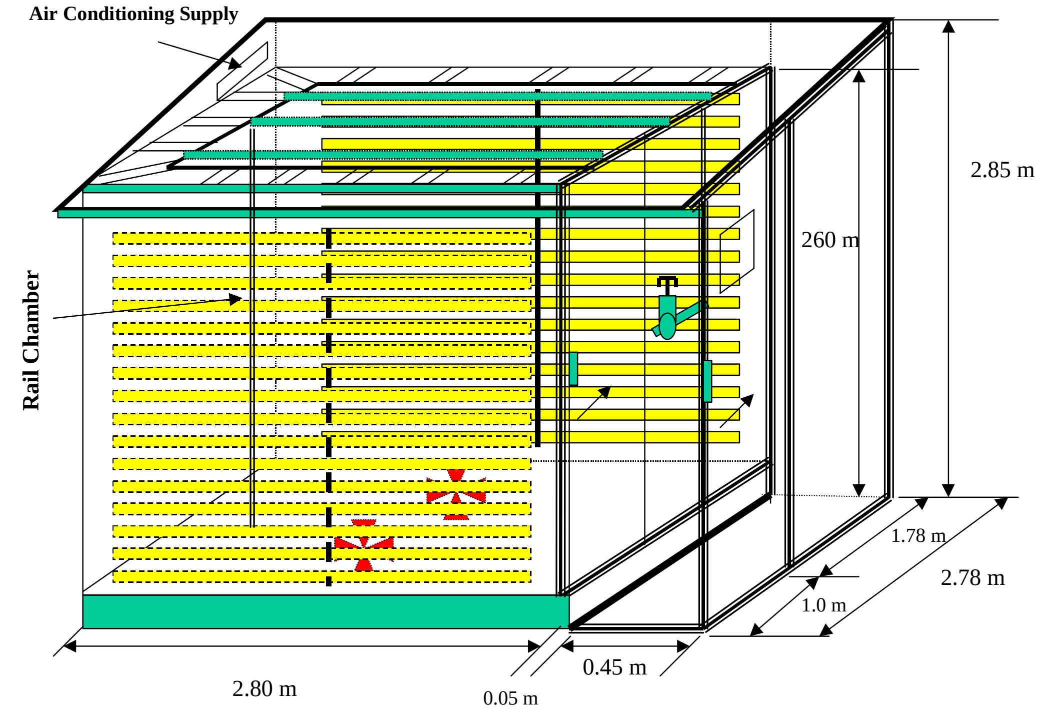
Appendix

This Appendix shows the layout and design of the new indoor environmental chamber laboratory being constructed at IMP, based on the results of the consultations carried out for this project.

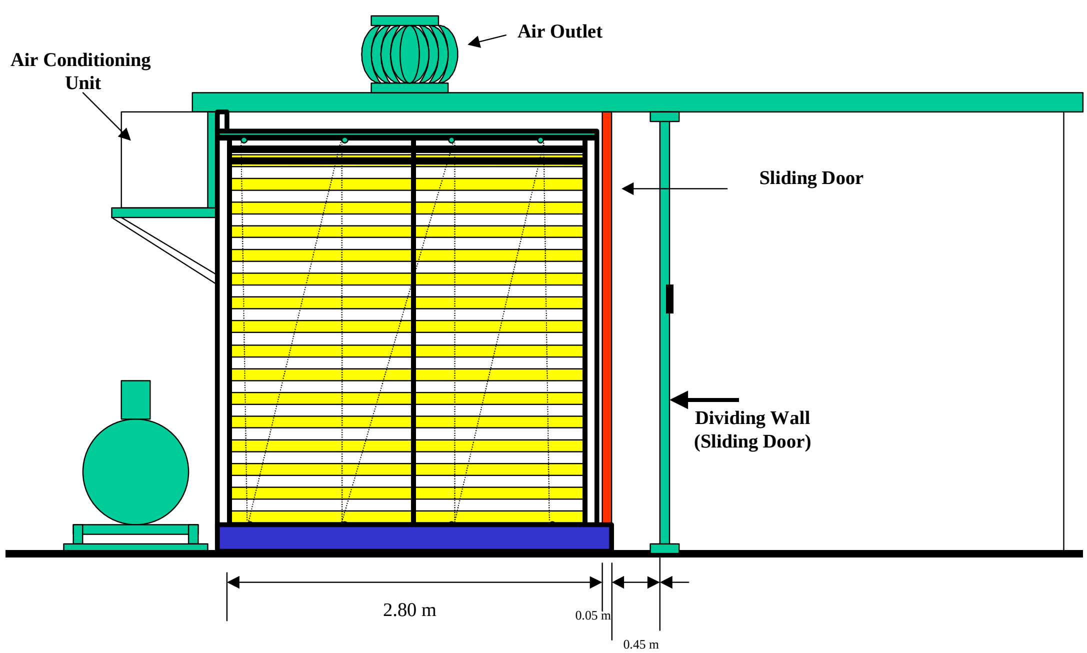
LAYOUT OF ENVIRONMENTAL SMOG CHAMBER LABORATORY



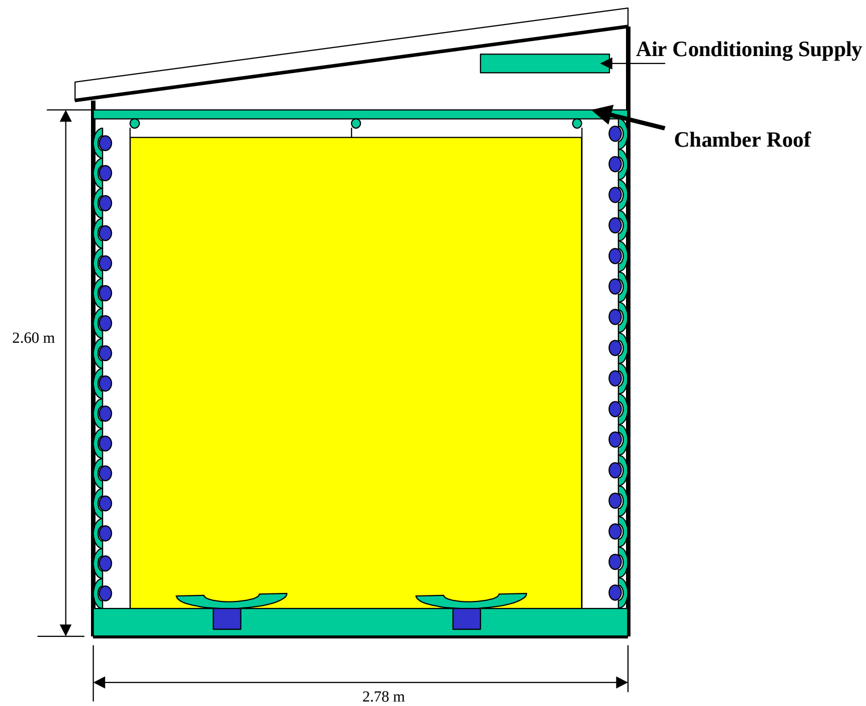
SMOG CHAMBER DESIGN



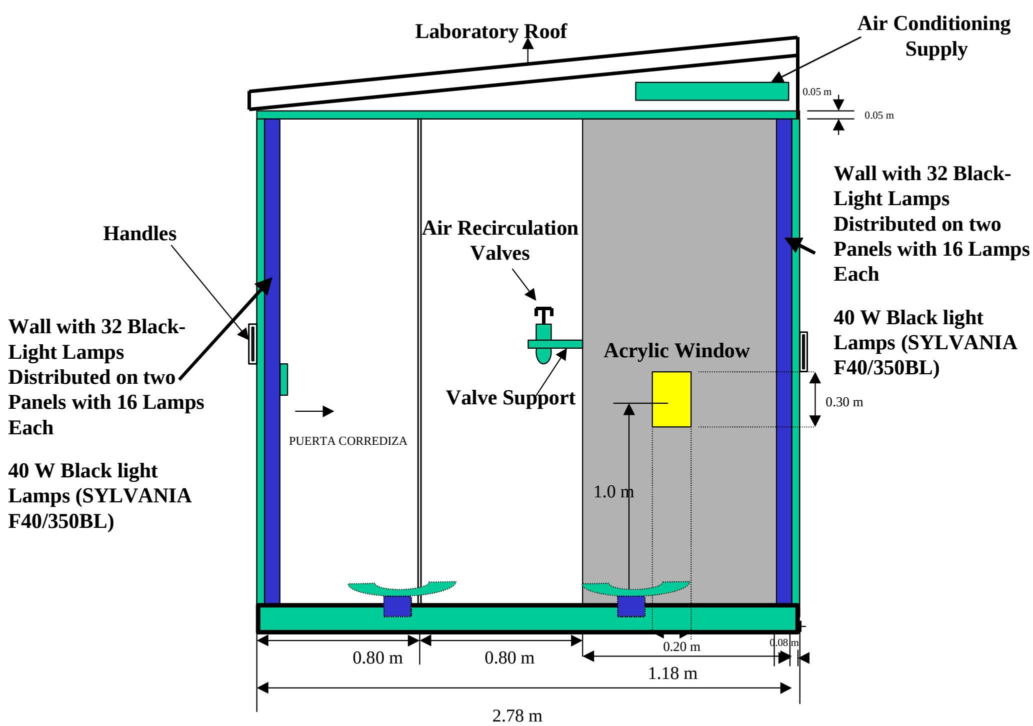
LEFT SIDE VIEW OF SMOG CHAMBER LABORATORY



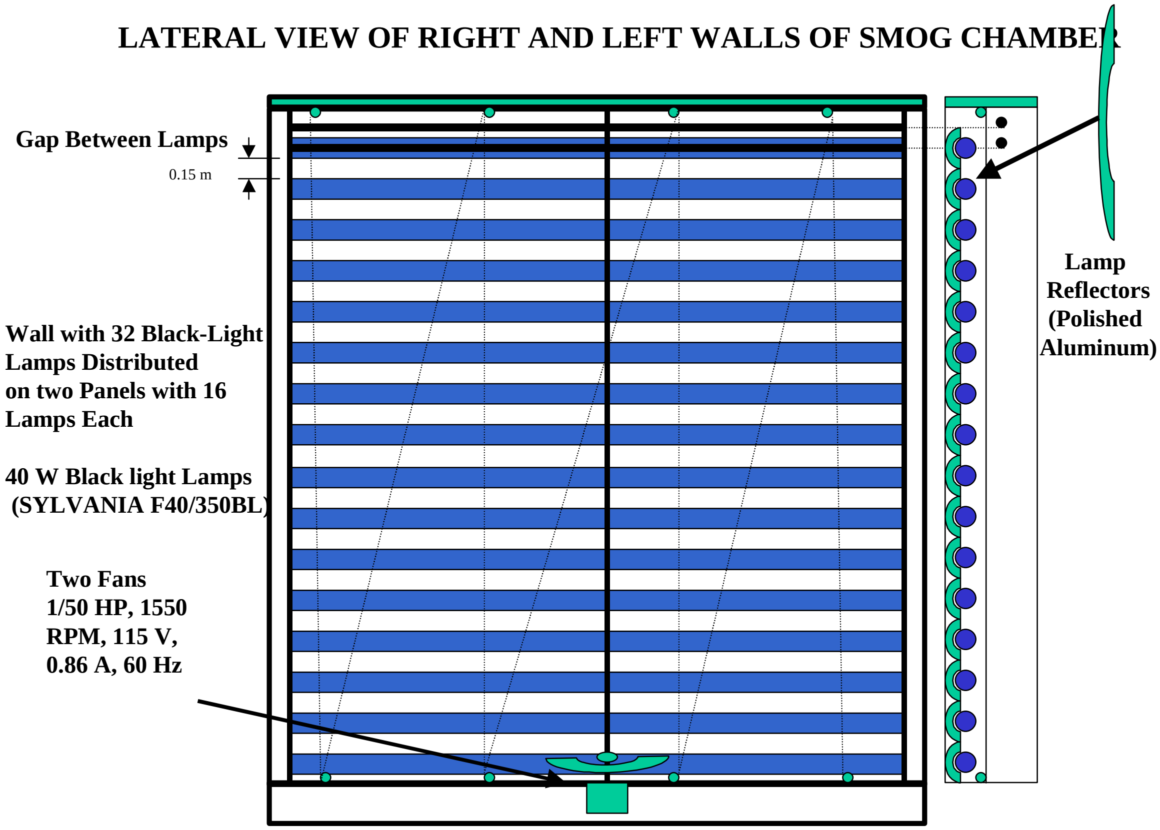
INTERIOR VIEW OF BACK WALL



FRONT VIEW OF THE MAIN ENTRANCE TO THE CHAMBER



LATERAL VIEW OF RIGHT AND LEFT WALLS OF SMOG CHAMBER



VIEW OF SMOG CHAMBER FLOOR FROM TOP