Evaluation of the Emission, Transport, and Deposition of Mercury, Fine Particulate Matter, and Arsenic from Coal-Based Power Plants in the Ohio River Valley Region

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PROJECT ABSTRACT

As stated in the proposal: Ohio University, in collaboration with CONSOL Energy, Advanced Technology Systems, Inc (ATS) and Atmospheric and Environmental Research, Inc. (AER) as subcontractors, is evaluating the impact of emissions from coal-fired power plants in the Ohio River Valley region as they relate to the transport and deposition of mercury, arsenic, and associated fine particulate matter. This evaluation will involve two interrelated areas of effort: ambient air monitoring and regional-scale modeling analysis.

The scope of work for the ambient air monitoring will include the deployment of a surface air monitoring (SAM) station in southeastern Ohio. The SAM station will contain sampling equipment to collect and measure mercury (including speciated forms of mercury and wet and dry deposited mercury), arsenic, particulate matter (PM) mass, PM composition, and gaseous criteria pollutants (CO, NO_x, SO_2, O_3, etc.). Laboratory analysis of time-integrated samples will be used to obtain chemical speciation of ambient PM composition and mercury in precipitation. Near-real-time measurements will be used to measure the ambient concentrations of PM mass and all gaseous species including Hg^0 and RGM. Approximately 18 months of field data will be collected at the SAM site to validate the proposed regional model simulations for episodic and seasonal model runs. The ambient air quality data will also provide mercury, arsenic, and fine particulate matter data that can be used by Ohio Valley industries to assess performance on multi-pollutant control systems.

The scope of work for the modeling analysis will include (1) development of updated inventories of mercury and arsenic emissions from coal plants and other important sources in the modeled domain; (2) adapting an existing 3-D atmospheric chemical transport model to incorporate recent advancements in the understanding of mercury transformations in the atmosphere; (3) analyses of the flux of Hg^0, RGM, arsenic, and fine particulate matter in the different sectors of the study region to identify key transport mechanisms; (4) comparison of cross correlations between species from the model results to observations in order to evaluate characteristics of specific air masses associated with long-range transport from a specified source region; and (5) evaluation of the sensitivity of these correlations to emissions from regions along the transport path. This will be accomplished by multiple model runs with emissions simulations switched on and off from the various source regions.

To the greatest extent possible, model results will also be compared to field data collected at other air monitoring sites in the Ohio Valley region, operated independently of this project. These sites may include (1) the DOE National Energy Technologies Laboratory's monitoring site at its suburban Pittsburgh, PA facility; (2) sites in Pittsburgh (Lawrenceville) PA and Holbrook, PA operated by ATS; (3) sites in Steubenville, OH and Pittsburgh, PA operated by the USEPA and/or its contractors; and (4) sites operated by State or local air regulatory agencies. Field verification of model results and predictions will provide critical information for the development of cost effective air pollution control strategies by the coal-fired power plants in the Ohio River Valley region.

EXECUTIVE SUMMARY

Ohio University is performing a Cooperative Agreement with the U.S. Department of Energy's National Energy Technology Laboratory (DOE-NETL) to conduct regional-scale modeling analysis and ambient air monitoring that will provide critical information for the development of relevant and cost effective control strategies by the coal-fired power plants in the Ohio River Valley region.

When the project is finished, researchers conducting the regional modeling studies will have developed a comprehensive budget of arsenic, elemental mercury (Hg^0), reactive gaseous mercury (RGM), and fine particulate matter across the Ohio Valley region, including sources, sinks, atmospheric lifetimes, burdens, and advective fluxes. In addition, updated emissions inventories for mercury and arsenic within the region will be developed to support the regional modeling studies. A comprehensive surface air monitoring (SAM) site is being developed and operated in southeastern Ohio to provide field data against which the model results can be compared. The SAM site has the capability of monitoring mercury speciation in ambient air and in precipitation, and it contains a full range of instrumentation for measuring the composition of fine particulate matter and co-pollutant gases. Short-term and seasonal simulations with the refined model are being compared to field measurements from the monitoring site, and the results are being used to develop a decision-support tool. A supplemental objective of the analysis is to evaluate the impacts of long-range transport from regions outside the Ohio Valley as well as biospheric recycling of elemental Hg on the measured and modeled reactive and total mercury concentration levels in the Ohio Valley region.

The Cooperative Agreement began in April of 2003. Two six-month no-cost extensions to the original 27 month performance period have been approved. This extends the project through December 2006. The effort has been broken down into the following seven separate tasks.

Task 1 consists of establishing and operating the SAM site in southeastern Ohio. Under this project, the SAM site has been set up; routine sampling was initiated on March 1, 2004; and data collection occurred through November of 2005.

Task 2 consists of the selection and evaluation of a 3-D regional-scale chemical transport model (CTM) for an application focused on the Ohio River Valley region. The Chemical Transport Model CMAQ (Community Multiscale Air Quality) model has been set up and is operational. A one-year base-case simulation has been completed for North America for the year 1996. The modeling system is currently being prepared for a 2004 base-case run. Model evaluation will be preformed with data collected from the Athens Supersite and the sensitivity evaluations will be completed with the 2004 base-case modeling system.

Task 3 involves the refinement and update of emission inventories (EIs) for sources of mercury and arsenic within and upwind of the modeled domain. The Institute for Sustainable Energy and the Environment (ISEE) plans to collect and process that emissions information into the model structure throughout the modeling effort.

Task 4 consists of making short-period model runs for comparison with field data. The summer of 2001 has been used for initial comparisons because of the extensive field data on particulate matter and co-pollutants available from the DOE-sponsored Pittsburgh Air Quality Study. The ambient monitoring fine particulate data (PM sulfate and PM nitrate) from the Pittsburgh site and other EPA-sponsored air quality sites have been used to calibrate the short-term atmospheric chemistry model (refer to Semi-Annual Technical Report # 3). The filter data from the Athens Supersite is currently being analyzed and will be used for model evaluation for the 2004 base-case run.

Task 5 involves seasonal-scale simulations focusing on the identification of significant sources and source regions contributing to the deposition of mercury and ambient concentrations of arsenic and fine particulate matter over periods of several months or more. As a part of accomplishing this task, the project team completed seasonal photochemical modeling simulations for the summer of 2004. This is the time period during which the SAM at Athens became operational. The quality and availability of these data are important in the decision-making processes and for confidence in the results arising from the air quality modeling applications. One of the significant components of this task is meteorological modeling simulations since the simulated meteorological variables are an essential input to the photochemical model. The research team has completed meteorological model simulations for the months of July-September, 2004. The results from this model evaluation were presented in the Semi-Annual Technical Report # 5. The research team is continuing to evaluate the meteorological model run against observational data sets to refine the accuracy of the model output. The modeling will also examine the efficacy of emission reduction strategies specifically for coal-fired power plants. In addition, researchers will conduct an analysis of long-range transport from regions outside the Ohio Valley as well as biospheric recycling of elemental Hg on the measured and modeled reactive and total mercury in the Ohio Valley region.

Task 6 consists of the development of Web-based model interface technologies to provide industry and government agencies with a user-friendly decision-support tool to facilitate the evaluation of source-receptor relationships and the efficacy of emission-reduction strategies. The framework for the Web-based GIS interface has been developed. Work on this task will continue throughout the remainder of this project.

Task 7 consists of project management, data analysis, and reporting functions. Specific accomplishments during this reporting period include 1) completion of the air monitoring field campaign, which includes sampling equipment for collecting and measuring mercury, arsenic, $PM_{2.5}$, pollutant gases, and weather data (the monitoring site is currently continuing under EPA funding); 2) continued refinement and updating of mercury and arsenic emission inventories for 2004; and 3) continued evaluation and refinement of the meteorological modeling for 2004.

I. INTRODUCTION

From the proposal: Ohio University is performing a Cooperative Agreement with the U.S. Department of Energy's National Energy Technology Laboratory (DOE-NETL) to conduct regional-scale modeling analysis and ambient air monitoring that will provide critical information for the development of relevant and cost effective control strategies by the coal-fired power plants in the Ohio River Valley Region.

Coal flue gas contains a variety of hazardous air pollutants (HAPs), including organic and inorganic chemical compounds. Among the latter, the metals mercury and arsenic are of particular concern because of their toxicity to humans and animals. An understanding of the chemistry of these elements should be the basis of proposed legislation to regulate mercury and arsenic emissions since specific chemical species will account for differences in human toxicity, rate of transport through the ecosystem, and the design variations in possible emission control schemes. An additional layer of complexity results from the fact that these elements may or may not be associated with fine particulate matter ($PM_{2.5}$ and PM_{10}) during or after emission from a stack. In general, the less volatile species such as arsenic and oxidized mercury are likely to be associated with fine particulate matter while the more volatile moieties such as elemental or reduced mercury tend to be emitted as non-associated gases. Thus, it will be necessary to determine the chemical forms of mercury and arsenic present at the stack and at designated receptor sites, and to determine the fractions of these species bound to fine particulate matter.

Mercury, fine particulate matter, and arsenic can be transported over large distances due to their minimal rate of sedimentation. In particular, mercury transport must be considered a global problem. Elemental mercury is believed to have a half-life of approximately one year in the atmosphere, and little is known about its cyclic transport between land, water, and air. Biogenic transport and biogenic sources are even less well understood. Therefore, the ISEE will adopt a regional scale approach for adequate evaluation of source-receptor relationships for mercury, fine particulate matter, and arsenic. Our approach in evaluating the impact of arsenic and mercury emissions from coal-fired power plants and other sources is to examine the source-receptor relationship through ambient monitoring and regional scale modeling.

A. Project Goal and Objectives

From the proposal: The overall objective of the project is to quantitatively evaluate the emission, transport, and deposition of mercury, fine particulate matter (PM), and air toxics (arsenic) in the Ohio River Valley region. This evaluation involves two interrelated areas of effort: regional-scale modeling analysis and ambient air monitoring.

The objective of the regional modeling studies is to develop a comprehensive budget of arsenic, elemental mercury (Hg^0) and reactive gaseous mercury (RGM), and fine particulate matter including sources, sinks, atmospheric lifetimes, burdens, and advective fluxes across the Ohio Valley Region. To support this objective, project researchers will develop updated emissions inventories for mercury and arsenic within the region. The second objective is to develop an air-monitoring site in Athens, Ohio to provide the capability to monitor mercury in ambient air and in precipitation. Researchers will compare the refined model's short-term and seasonal simulations to field measurements from the monitoring site and use the results to develop a decision-support tool. A supplemental objective of the analysis is to evaluate the impacts of long-range transport from regions outside the Ohio Valley as well as biospheric recycling of elemental Hg on the measured and modeled reactive and total mercury concentration levels in the Ohio Valley region.

B. Project Development (Tasks)

Seven separate tasks are to be completed over the 33-month performance period. (Two six-month no-cost extensions to the original 27 month performance period have been requested and approved.) The following project schedule is based on a project start date of April 3, 2003. Table 1 on page 3 presents a progress summary for each task. Section II Experimental Design is a detailed description of each task and the progress achieved toward its completion as of April 2, 2006.

Project Schedule

- Task 1 consists of establishing and operating a Stationary Ambient Monitoring (SAM) site in Athens, Ohio. Routine sampling was initiated on March 1, 2004 and continued through November, 2005.

  (Tasks 2–6 comprise the modeling process, which will continue throughout the project. Throughout Tasks 2–6, the project team will keep abreast of ongoing research and newly published literature pertaining to the atmospheric behavior of mercury. Whenever possible, new findings concerning mercury speciation and transport will be incorporated into the model algorithms.)

- Task 2 consists of the selection and evaluation of a 3-D regional-scale chemical transport model (CTM) for an application focused on the Ohio River Valley region. The project team has completed the setup and development of the CTM grid system and conducted a one-year base-case simulation for North America for the year 1996. Currently the modeling system is being configured for a 2004 base case run.

- Task 3 involves the refinement and update of EIs for sources of mercury and arsenic within and upwind of the modeled domain. The project team anticipates that information on emissions will continue to be collected and processed into the model structure throughout the modeling effort. In addition, researchers will update the EI for mercury with new China emissions data developed by David Streets of the Argonne National Laboratory.

- Task 4 consists of conducting short-period model runs for comparison with field data. A short-term modeling run has been completed for July 2001 for the eastern United States. The model run was conducted with the photochemical model CMAQ. For initial comparisons, the project team used particulate sulfate and nitrate data collected during the summer of 2001 from the DOE-funded Pittsburgh Air Quality Study. In addition, the team will conduct short-term model runs for comparison with the speciated mercury and arsenic data collected at the Athens SAM for the 2004 sampling periods.

- Task 5 involves seasonal-scale simulations that focus on the identification of significant sources and source regions contributing to the deposition of mercury and ambient concentrations of arsenic and fine particulate matter over periods of several months or more. As a part of this ongoing process, the project team has set up meteorological model MM5 model simulations for the summer of 2004 (refer to Semi-Annual Technical Report #5). Currently, the MM5 output is being evaluated against observational data sets. The modeling will also examine the efficacy of emission reduction strategies specific to coal-fired power plants. In addition, researchers will analyze the long-range transport from regions outside the Ohio Valley and the biospheric recycling of elemental Hg on the measured and modeled reactive and total mercury in the Ohio Valley Region.

- Task 6 consists of the development of Web-based model interface technologies to provide industry and government agencies with a user-friendly decision-support tool to facilitate the evaluation of source-receptor relationships and the efficacy of emission reduction strategies. The framework for the GIS Web interface has been completed. The development of the Web-based system will continue through the remainder of this project.

- Task 7 consists of project management, data analysis, and reporting functions.

Table 1 below is a progress summary for each task.

Table 1. Progress summary

Task #	Description	Planned % Completed	Actual % Completed
1	SAM	100	100
2	Base Case Simulation	100	100
3	Emission Inventories	100	90
4	Model Comparison	100	70
5	Seasonal Scale Simulations	100	40
6	Development of Support Tool	100	40
7	Project Management	100	70

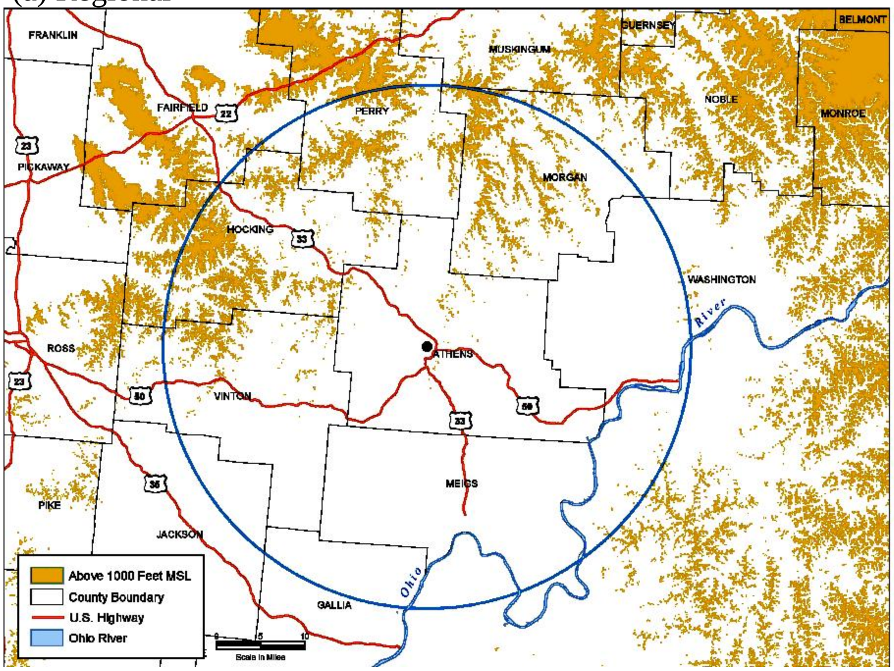
II. EXPERIMENTAL DESIGN

In this section, the description of each task is presented as it was proposed in the funding application. Following the description is a discussion of the progress made toward completing the task.

Task 1. Establish and operate a (SAM) station in Athens, Ohio

The proposal for this project designated that the ISEE would establish a SAM station in Steubenville, Ohio. However, prior to April 3, 2003 the Environmental Protection Agency set up a SAM station in Steubenville that has the capacity to monitor for mercury. Consequently, the ISEE was able to select another site for the SAM station proposed for this project. The project staff located an optimal site south of Athens, Ohio in the heart of the Ohio River Valley. At an elevation of 950 feet, the site is the highest point within a 100-mile radius to the east, south, and west (Figure 1, page 4). It is an excellent site from which to capture the transport of pollutants into and out of the valley.

(a) Regional



(b) Local

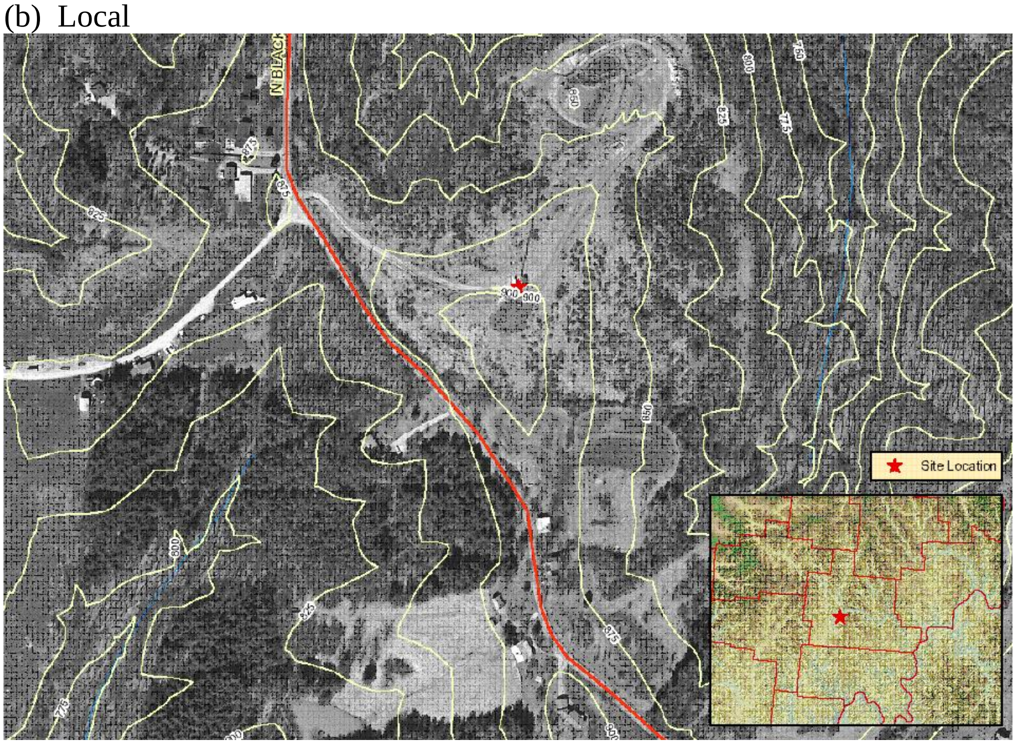


Figure 1. Topographical map of the Athens site: (a) regional and (b) local

The Athens site utilizes air-monitoring equipment from the Steubenville Comprehensive Air Monitoring Project (SCAMP), sponsored by DOE-NETL under Cooperative Agreement DE-FC26-00NT40771. In addition, the site includes sampling equipment for collecting and measuring mercury, including total, elemental, reactive, particulate, and wet/dry deposition.

Task 1: Ambient monitoring accomplishments from October 3, 2005 to April 2, 2006:

Three primary objectives during this period were to

- Maintain instrument operation
- Enhance data QA/QC recovery
- Disseminate preliminary data by attending conferences and preparing publications

Accomplishments by month:

October

- Gas analyzers, with the exception of O_3, operated properly all 31 days in October. Maintenance included the replacement of the savillex filters. The performance of the analyzers was checked every two days by comparing the calibration drift to the acceptable limits.

- The Tekran experienced a problem known as gold trap passivation, in which water in the zero air tanks effectively removed mercury from the sample stream. Tekran data collection was suspended from Oct. 14–Oct. 20 so that the proper materials could be acquired for solving this problem.

- Rainwater collection for analysis of mercury concentration was successful on 4 out of 4 weekly attempts.

- There were no problems with the TEOM, FRM, or speciation samplers during October 2005. Technicians changed the filters when necessary.

November

- Valid collection of continuous gases, with the exception of O_3, continued through November 16, 2005. After this date, the Model 700 calibrator was removed from the system for repair. SO_2, NO_x, and CO analyzers continued to operate to the end of the month without daily span and zero checks. The remainder of this data is considered "flagged" until the November 30, 2005 collection end date.

- The Tekran produced valid mercury data on 29 of out 30 days in November 2005. Regular maintenance including calibrations and denuder replacement occurred as recommended. Data collection for this project ended November 30, 2005.

- The TEOM, FRM, and speciation samplers operated throughout November until data collection ended on November 27, 2005. FRM and speciation filters were canceled on Nov. 27, 2005; however, that sample was rescheduled for Dec. 3, 2005, which served as the end date for these two samplers. Maintenance on the FRM and speciation samplers included recalibration, cleaning of the PM inlet, and fan filter replacement on Nov. 17.

December-March

Under the DOE contract the ambient monitoring was concluded in November 2005. The site is currently being expanded under an EPA contract to include the installation of a NOy, low level CO, and additional equipment to support regional haze evaluations. Consol Energy R&D will continue to analyze the filter samples generated over the last 18 months and researchers at the Air Quality Center will continue to perform data reduction and QA/QC on all the sampling data (Tekran, TEOM, gases, meteorological, mercury deposition, FRM, and speciation).

Additional Items

- Contributions by Ohio University and CONSOL Energy R & D led to the following publication, submitted to *Atmospheric Environment* for initial review in October 2005:

  Reddy Yatavelli, Jason Fahrni, Myoungwoo Kim, Kevin Crist, Chris Vickers (Ohio University), Steve Winter, and Daniel Connell (CONSOL). "Mercury, Pm2.5 and Gaseous Co-Pollutants in the Ohio River Valley Region: Preliminary Results from the Athens Supersite."

  In February 2006, the *Atmospheric Environment* review was complete and the document was in its final phase of editing by Ohio University/ CONSOL Energy R & D.

- Ohio University and Consol Energy R & D are currently preparing a manuscript titled "The Episodic Nature of Ambient Mercury at a Rural Ohio River Valley Supersite."

- As of the end of March 2006, the following analytical activities were completed:
  - Approximately 60 denuders have been coated for mercury sampling.
  - More than 1,000 filters have been pre- and post-weighed for PM sampling.
  - ~325 quartz filters were analyzed for carbon species.
  - ~135 Teflon filters were extracted and analyzed for ions.
  - ~100 filters were analyzed for trace elements.

<u>Task 2. Evaluate and Select a 3-D Regional-Scale Atmospheric Chemical Transport Model (CTM) and Conduct a Base-Case Simulation</u>

Several 3-D regional-scale CTMs with the ability to simulate tropospheric ozone, visibility, and fine particulate matter are appropriate for application to the Ohio River Valley region to evaluate total fine particulate matter mass and the arsenic component of fine particulate matter. The ISEE and Atmospheric and Environmental Research (AER) have established the 3-D modeling framework. AER completed a base-case model simulation for the year 1996.

The project team chose the Community Multi-Scale Air Quality (CMAQ) model for air-pollution studies on a regional scale for this study. The EPA and its collaborators (Byun &

Ching, 1999) developed the CMAQ, which uses non-hydrostatic Penn State/NCAR mesoscale model (MM5) V3-derived dynamics for transport.

Task 2 accomplishments through April 2, 2006

- Conducted an annual simulation for 1996 using the modified CMAQ-Hg code with the MEBI chemistry solver. The modeling year was divided into four 3-month periods (Jan–Mar, Apr–Jun, Jul–Sep, Oct–Dec) and 3-month simulations were conducted on different processors to speed up the overall completion of the annual simulation. A 10-day spin-up cycle was used for each 3-month simulation period. Each simulation day requires about 3 hours of CPU time.

- The seasonal boundary conditions from the global mercury chemistry transport model were applied as follows for the 3-month simulation periods:

➢ Winter boundary conditions: January, February, and December

➢ Spring boundary conditions: March, April, and May

➢ Summer boundary conditions: June, July, and August

➢ Fall boundary conditions: September, October, and November

- The version of the CMAQ-Hg code used in these simulations also included modifications to calculate and save the daily cumulative dry and wet deposition amounts and daily average concentrations of Hg. (The default model saves only the hourly values).

The results from the model evaluation of CMAQ-Hg for 1996 annual simulations were presented in the semi-annual technical report #3. The appraisal of the model was done solely on the basis of the wet deposition flux the observations of which were obtained from the mercury wet deposition sites.

The project team plans to carry out further air quality modeling simulations for the summer of 2004. Additionally, researchers will measure the output from this CMAQ-Hg model run against observations of elemental, reactive, and particulate mercury from the DOE-NETL-sponsored observational sites at Athens and Steubenville. This will enable them to understand whether the model can reasonably quantify the atmospheric mercury levels in addition to acceptably estimating the deposition fluxes.

The emissions input to the new CMAQ-Hg runs for 2004 will include an enhanced global emissions inventory consisting of a new emissions inventory of mercury for China, which is a supposedly high emitter of mercury. The China inventory, coupled with an innovative global model, will provide a fresh assessment of the relative contributions of local and distant sources to mercury deposition in Ohio.

Finally, a new version of CMAQ-Hg will be used for the 2004 modeling simulations. Five new sources of mercury emissions from natural sources have been added to the modified Community Multiscale Air Quality-Mercury (CMAQ-Hg) modeling system. An annual deposition of mercury from a previous CMAQ simulation was used to develop an annual inventory for "recycled" oceanic and land-mercury emissions. Likewise, these two inventories were scaled based on solar radiation and temperature. Code was developed to create model-ready emissions for these five sources. This new version of CMAQ-Hg will become operational in 2006. Currently the research team at Ohio University is developing the modeling framework for the 2004 base case. The model simulations will be performed in a nested mode with a horizontal grid-cell dimension for the finest grid system of 4 km in a domain consisting of Ohio. For the remainder of the modeling domain covering the continental United States, a 12-km and 36-km grid system will be used (Figures 1 and 2). The vertical structure in the model consists of 14 layers from the surface up through 4 km. The base-case run will be continuously modified to improve prediction accuracy in the model calibration step.

The Sparse Matrix Operator Kernel Emission Model (SMOKE) is being used to process the emissions inventory for the model-ready input. The model is temporally and spatially processing the 2002 National Emissions Inventory (NEI) and the Ohio Emissions Inventory (Base L Inventory—the most current EI for 2002). The Base L inventory, prepared by the Lake Michigan Air Directors Consortium (LADCO), consists of elevated point source, low-level point source, area, and non-road sources. As for the on-road sources, researchers are using the most current inventory, the Base L Inventory of on-road sources. The Ohio EI files are composed of weekday, Saturday, and Sunday in gridded emission files for each month. Project personnel are using spatial analysis tools in the GIS for spatial allocation of emissions sources to proper grids. Proper emission surrogates are identified and developed for the allocation of emission sources.

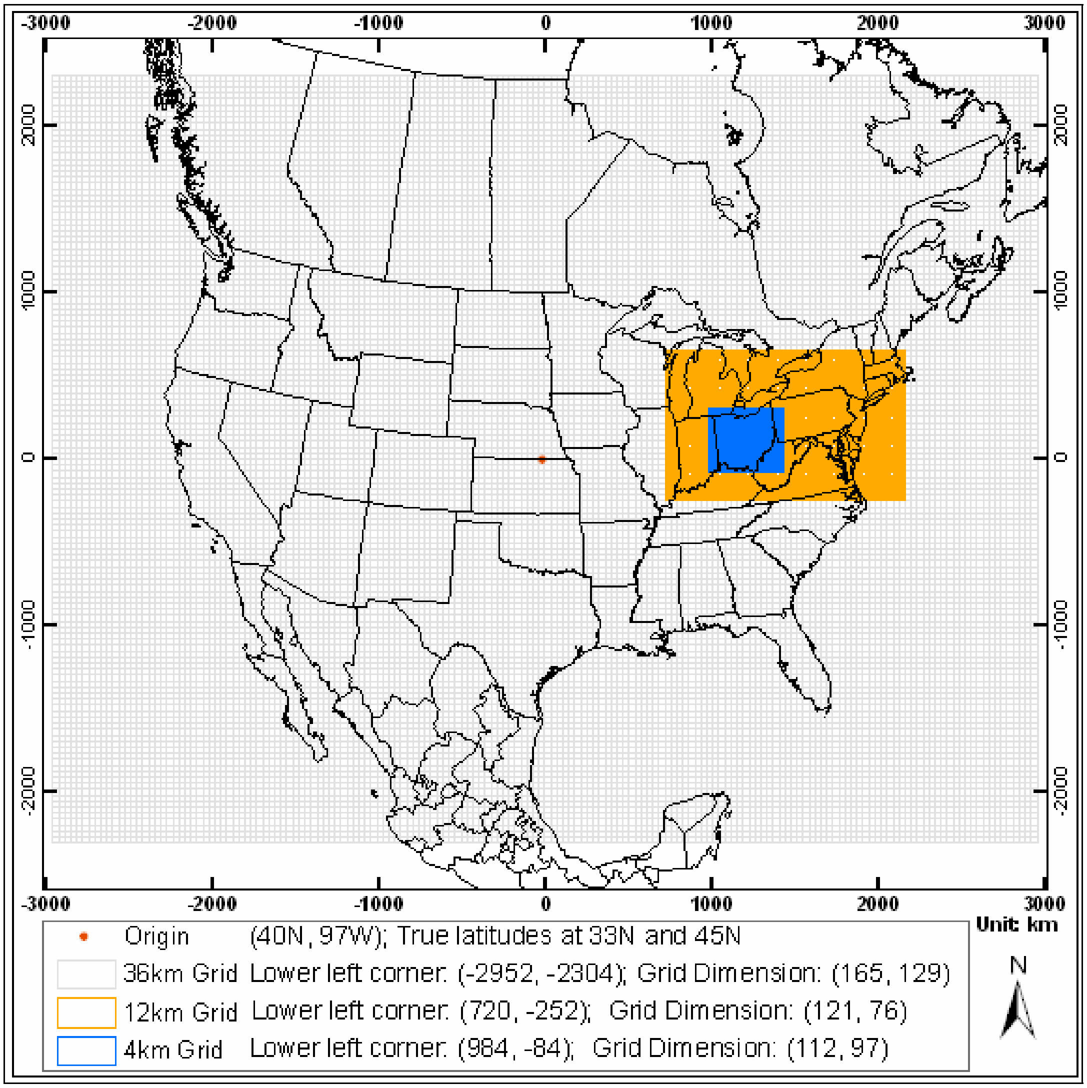


Figure 2. Modeling Domain and Nested Grids in Lambert Conformal Projection (LCP)

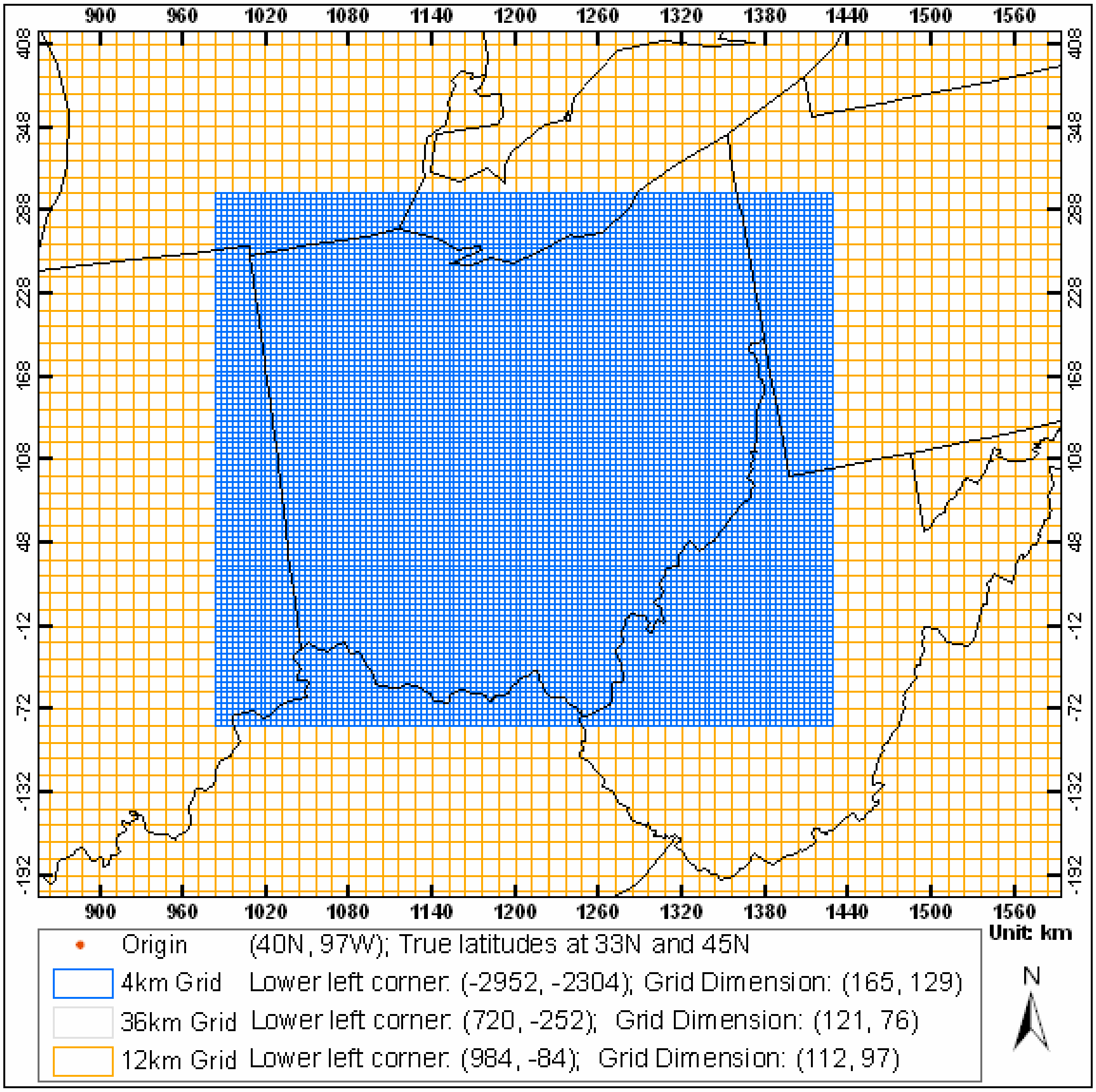


Figure 3. 4-km nested grid in Lambert Conformal Projection (LCP)

Task 3. Refine and Update Emission Inventories (EIs)

Proposed: Ohio University and Advanced Technology Systems, Inc. (ATS) will enhance the mercury and arsenic emission inventories.

Task 3 accomplishments from October 3, 2005 to April 2, 2006:

- The research team continued the refinement of the mercury emissions. ATS is currently working with Ohio University to integrate the updated mercury emissions into the emission inventories for CMAQ simulations.

- Project researchers are currently working under a separate project with David Streets at the Argonne National Laboratory to incorporate updated China Emissions for the global model.

<u>Task 4. Perform Short-Period Model Runs for Comparison with Field Data</u>

Proposed: ISEE will conduct a series of model runs to evaluate the system against field observations. The model run will correspond to the NETL-sponsored intensive sampling campaigns centered in Pittsburgh, Pennsylvania. Researchers will combine the extensive datasets collected during this campaign with other relevant datasets in this region. Meteorological input data for these simulations will be derived diagnostically using MM5 V3. The model evaluations involve short-time-period runs for the field-intensive periods, storing hourly averaged fluxes and production-and-loss rates for ozone, hydrocarbons, arsenic, Hg^0, and RGM for direct comparison with field data. In addition, long-range transport events will be identified from the short-term CTM runs and evaluated with the observational data set.

In addition to the model evaluations conducted from field observations obtained from the 2001 NETL-sponsored sampling campaigns, the model will be evaluated against the observational data sets, including the speciated mercury and arsenic data collected at the Athens SAM for the 2004 sampling period. These simulations will be vital for model verification because the Athens SAM will be one of the few sites providing measurements on individual mercury species and arsenic. The model evaluations involve short-time-period runs for the field-intensive periods, storing hourly averaged fluxes and production-and-loss rates for ozone, hydrocarbons, arsenic, Hg^0, and RGM for direct comparison with field data. In addition, long-range transport events are identified from the short-term CTM runs and evaluated with the observational data set.

Task 4 accomplishments through April 2, 2006:

- Work is underway to perform regional and urban modeling simulations for 36-, 12-, and 4-km-grid resolutions for the year 2004 (refer to description in task 2). The 36-km grid will cover most of Eastern United States, whereas the 4-km domain will cover all the power plants in the Ohio River Valley region.

- The chemical transport model CMAQ has been evaluated using hourly and mean particulate sulfate and nitrate observations for the time period of July 2001. The hourly sulfate and nitrate observational data were obtained from the DOE-sponsored super site at Pittsburgh, and the mean sulfate and nitrate data were obtained from EPA-sponsored air quality sites in and around the Pittsburgh region.

- The meteorological inputs were obtained from EPA's 2001 MM5 simulations and the processed emission inputs were based on EPA's 2001 National Emissions Inventory. The spatially and temporally varying lateral boundary conditions for each day of the modeling simulation were obtained from EPA. These boundary conditions were generated by EPA using a global atmospheric model.

Task 5 - Seasonal Scale Simulations

Proposed: A major focus of the modeling effort is to identify significant sources and source regions contributing to the deposition of mercury and ambient concentrations of arsenic and fine particulate matter. The modeling will also examine the efficacy of reduction strategies specifically for coal-fired power plants. In addition, researchers will conduct an analysis of the long-range transport from regions outside the Ohio Valley and the biospheric recycling of elemental Hg on the measured and modeled reactive and total mercury in the Ohio Valley Region.

Initially, researchers will set up a seasonal scale simulation for the entire North American continent on a coarse grid (36 km x 36 km), with a nested grid of 12 km over the Midwestern region of the United States and 4 km over the Ohio Valley Region. They will use the NCEP-4D assimilation data set to drive the regional-scale meteorology model (MM5 V3) to develop dynamic inputs for the CTM. The model analysis will be completed for the seasonal run to establish a 'base-case' simulation or the most likely current-day simulation for the season. Uncertainty ranges will be developed for critical parameters in the model, such as emissions and deposition rates. Additional seasonal scale simulations will be performed to develop an 'uncertainty envelope' of the model-generated estimates of deposition rates and fluxes.

Task 5 accomplishments through April 2, 2006:

- The research team is currently preparing for the 2004 sensitivity evaluations (task 2 and 4). The schematic for the evaluations is depicted in Figure 4.

- The project team is also developing the modeling framework for the 2004 run. The sensitivity analysis will be completed as soon as the system has been established and evaluated against observational data sets.

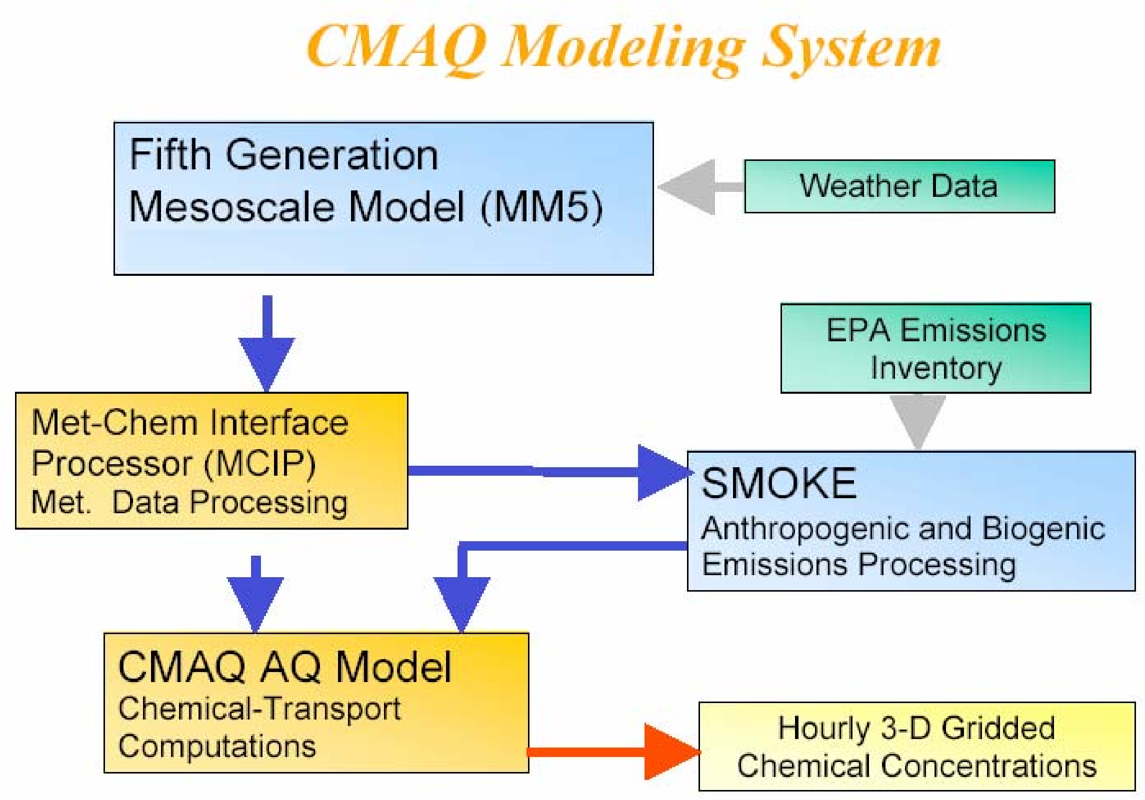


Figure 4. CMAQ modeling system

Task 6. Development of a Decision-Support Tool

Proposed: ISEE will conduct a series of model runs to perform a matrix analysis of the sensitivity of point sources to deposition patterns in the region. The analysis will also include selective emission reduction scenarios for these point sources. The team will couple this matrix with a GIS and the emission pre-processor to provide a detailed spatial analysis of the source–receptor relationships. In addition, this entire system will be supported by Web-based technologies to provide industry and government agencies with a user-friendly decision-support tool that will evaluate source-receptor relationships and the efficacy of emission reduction strategies.

Task 6 accomplishments through April 2, 2005:

Researchers have completed the framework for the Web-based support tool. They developed an interactive Web based GIS interface linking sources with a database that will contain the results from the matrix analysis. The Web-based system will provide a user-friendly interface linking specified source reductions with the associated impact on receptor sites.

Task 7. Project Management, Data Analysis, and Reporting

Proposed: This task involves all communication between the project team members, DOE-NETL, and external collaborating parties and includes all meetings, presentations, and

DOE-required reports pertaining to the project. To facilitate data analysis, the data from the SAM and the results of the model runs will be archived into a user-friendly database that will provide functionality to help calculate final mercury, arsenic, and fine particulate matter mass and composition concentrations. It will also allow the delineation of basic trends and the evaluation of variables. To the greatest extent possible, the data from the SAM site will be incorporated into the ambient air quality database being compiled for DOE-NETL by ATS and Ohio University under project DE-FC26-02NT41476. However, the primary function of the database will be to reduce data efficiently for evaluation of the proposed model simulations. At the conclusion of the project, Ohio University will submit the database containing the SAM information, results of model runs, and comparison statistics to DOE-NETL along with a comprehensive final report.

Task 7 accomplishments from October 3, 2005 to April 2, 2006:

- An extended abstract for an oral presentation on preliminary findings from the Athens Supersite was accepted for the AWMA National Conference in June of 2006.

- Researchers completed the monitoring campaign at the Athens Supersite under this contract. The site is supported under a separate EPA contract. At present, the research team is completing the analysis of the speciation samples (Consol Energy R&D) and reducing the data set for final analysis and to support the modeling efforts.

- Ohio University and Consol R&D submitted a paper detailing the initial phase of sampling to *Atmospheric Environment*. The paper was accepted and is undergoing final revisions.

III. SUMMARY OF RESULTS

The monitoring campaign at the Athens SAM was concluded in November of 2005 under this contract. The site is currently in operation under an EPA contract and has been expanded to include NOy, low level CO (used as co-pollutants for mercury source and transport analysis), and measurements for regional haze. Consol R&D is conducting the $PM_{2.5}$ speciation filter analysis and Ohio University is completing data reduction and QA/QC on the entire data set.

The ISEE researchers chose the CMAQ model developed for air-pollution studies on a regional scale by the EPA and its collaborators. AER has accomplished the 1-year run for the 36-km-grid domain for 1996 using CMAQ. Model performance for the 1996 simulation was conducted by comparing predicted annual wet deposition fluxes with 1996 data from the Mercury Deposition Network. The modeling framework for the 2004 base-case simulation is currently underway and will be completed later this year. The sensitivity analysis, identifying significant sources and source regions contributing to the deposition of mercury, will be conducted when the 2004 base-case simulation is completed.

ATS and Ohio University are continuing to upgrade the mercury and arsenic emission inventory files. The focus of their efforts is to develop a comprehensive and accurate emission inventory utilizing current research on emissions data from coal-fired power plants. The ISEE has initiated work on the short-scale simulations for 2004 and developed a GIS interface for the decision support tool.

Argonne National Laboratory is currently engaged in developing an enhanced global emissions inventory for mercury which will include a recently completed DOE/NETL inventory of emissions in China which was funded under a separate project and will be utilized in this study.

The research team from the Air Quality Center at Ohio University has presented preliminary results from a month of MM5 simulation (July, 2004). The model predicts temperatures, winds, and humidity with reasonable accuracy but over-predicts precipitation to a large extent. Sensitivity runs were also carried out for short time periods to determine the cumulus parameterization scheme best equipped to simulate precipitation for this particular modeling simulation. Currently the research team is conducting observation nudging to enhance model predictions.

IV. CONCLUSIONS

The research team has concluded the monitoring campaign. The team is now focusing on data reduction and analysis and completing the analytical activities associated with the $PM_{2.5}$ speciation and FRM samples. The modeling framework for the 2004 base-case simulation is currently being developed and will be used for the sensitivity analysis.

REFERENCES

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