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

Semi-Annual Technical Progress Report
for the Period April 3, 2004–October 2, 2004

to

Department of Energy
Washington, D.C.

DOE Award Number: DE-FC26-03NT41723

Award Recipient:

Ohio University
Athens, Ohio

Report Period Start Date:	April 3, 2004
Report End Date:	October 2, 2004
Principal Author:	Kevin Crist Ohio University
DOE Award Number:	DE-FC26-03NT41723
Contractor:	**Ohio University** Institute for Sustainable Energy and the Environment Building 21, The Ridges Athens Ohio, 45701
Subcontractors:	**CONSOL Energy** Research & Development 400 Brownsville Road South Park, PA 15129-9566 **Advanced Technology Systems, Inc.** 639 Alpha Drive—RIDC Park Pittsburgh, PA 15238-2819 **Atmospheric and Environmental Research, Inc.** 131 Hartwell Avenue Lexington, MA 02421-3126

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PROJECT ABSTRACT

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, NOx, 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 of 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 Hg0, 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 U.S. EPA 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.

The regional modeling studies will develop 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. 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 has the capability to monitor 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 will be compared to field measurements from the monitoring site, and the results will be 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. A six month no cost extension to the original 27 month performance period has been requested. This would extend the project through December of 2005. The effort has been broken down into seven separate tasks as follows:

Task 1 consists of establishing and operating the SAM site in southeastern Ohio. The SAM site has been set up and routine sampling was initiated on March 1, 2004; data collection will occur over the following 18 months. An overview of data obtained from the site through October 2, 2004 is presented in Section II (Experimental Design).

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. An analysis of the base case simulation will be completed and presented in the next semi-annual report.

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 short-period model runs to be made 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. Short-term model runs for comparison with the speciated mercury and arsenic data collected at the SAM for the 2004 sampling periods will follow these initial comparisons.

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. 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 and 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.

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

Accomplishments and tasks completed during this reporting period include (1) conducting a one-year base case simulation for the year 1996 with the 3-D chemical transport model (2) performing short-term photochemical modeling simulations during the month of July for the year 2001 and evaluating model output simulations with regards to observations from the DOE sponsored Pittsburgh Air Quality Study. (3) continued to refining and updating mercury and arsenic emission inventories for 2004; (4) operating a surface air monitoring station (SAM) at Athens, Ohio which includes sampling equipment for collecting and measuring mercury, arsenic, $PM_{2.5}$, pollutant gases, and weather data over the project period.

I. INTRODUCTION

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

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 will be completed over a 33-month performance period. A six month no cost extension to the original 27 month performance period has been requested. 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 October 2, 2004.

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. Data collection will occur over the following 18 months.

Tasks 2–6 comprise the modeling process, which will continue throughout the first 30 months of 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 a one-year base-case simulation for the year 1996 has been conducted for North America.

- Task 3 involves the refinement and update of emission inventories (EIs) for sources of mercury and arsenic within and upwind of the modeled domain. It is anticipated that information on emissions will continue to be collected and processed into the model structure throughout the modeling effort.

- 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. The project team used particulate sulfate and nitrate data collected during the summer of 2001 from the DOE funded Pittsburgh Air Quality Study for initial comparisons. In addition short-term model runs for comparison with the speciated mercury and arsenic data collected at the Athens SAM for the 2004 sampling periods will be conducted.

- 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.

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 will consist 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.

- 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	75	50
2	Base Case Simulation	100	50
3	Emission Inventories	100	66
4	Model Comparison	100	50
5	Seasonal Scale Simulations	0	0
6	Development of Support Tool	0	0
7	Project Management	75	33

II. EXPERIMENTAL DESIGN

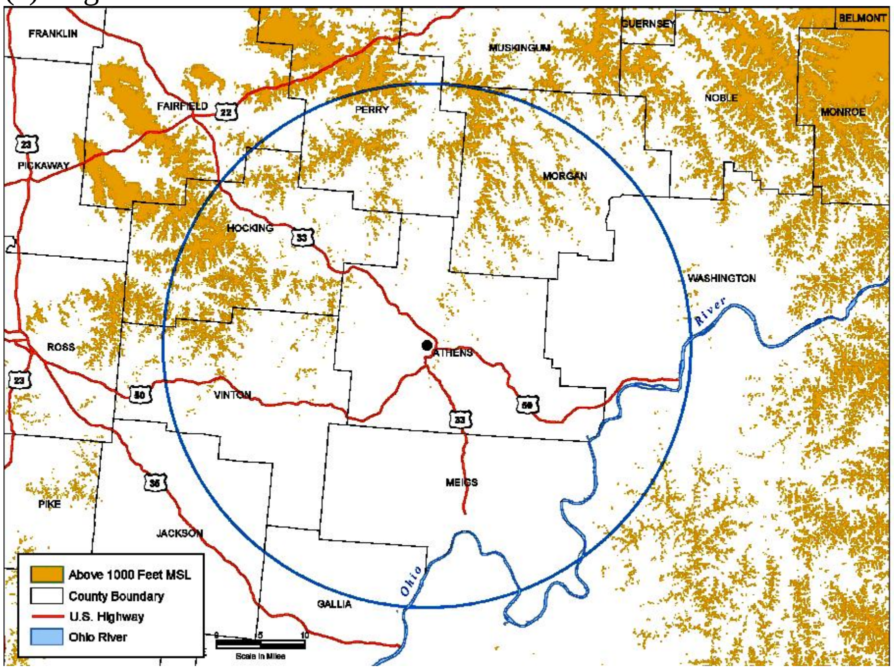
In this section, the description of each task is presented as it was proposed in the funding application. Following the description is a discussion of the progress made toward completing the task.

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. In addition, a 350-foot communication tower is adjacent to the site. ISEE has installed a wind-speed and wind-direction sensor atop the tower that will provide critical information for evaluating transport events.

NOTE: Consol Energy R&D is involved with Task 1 under subcontract to Ohio University. The subcontract was not executed until August 5, 2003, which delayed Task 1 by several months.

(a) Regional



(b) Local

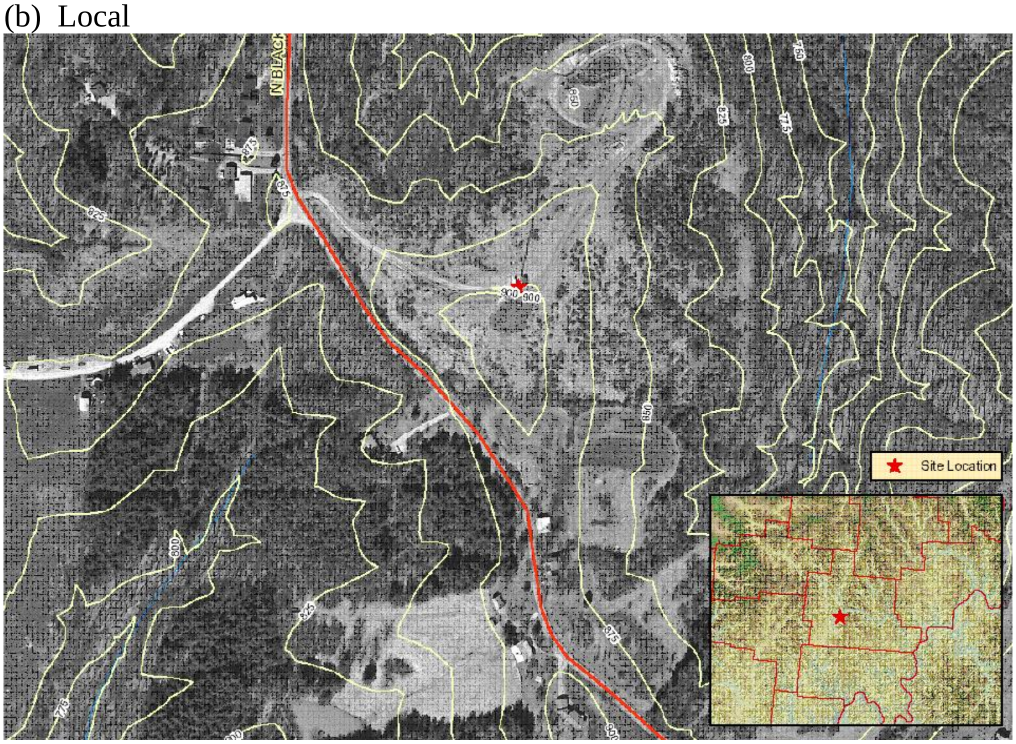


Figure 1. Topographical map of the Athens site: (a) regional and (b) local

The Athens site utilizes air-monitoring equipment from the NETL-sponsored SCAMP. In addition, the site includes sampling equipment to collect and measure mercury, including total, elemental, reactive, particulate, and wet/dry deposition.

Task 1 accomplishments from April 3, 2004 to October 2, 2004:

There were two primary objectives during this period:

- Maintain instrument operation
- Enhance data QA/QC recovery

Accomplishments: By month

- **April**
  - A security fence at the monitoring site was erected.
  - Sampling was initiated at the site which included: the federal reference method (FRM) $PM_{2.5}$ filter-based and $PM_{2.5}$ speciation sampler, the SO_2, O_3, CO and NO_x ambient gas analyzers and the TEOM Series 1400a Ambient Particulate Monitor. The Tekran, which includes the modules for analysis of reactive gas, elemental and particulate mercury, was also setup and brought online.
  - There was a strong collection of mercury wet deposition data and corresponding meteorological data during the month. However the Tekran malfunctioned during the last week of April.
  - The wet deposition sampler was moved off the sampling deck to the ground at the request of the Illinois Water Survey. The wet deposition sampler was accepted into the Mercury Deposition Network.
- **May**
  - A wind speed wind direction monitor was installed on the adjacent communication tower at 400ft.
  - Continued to work on the Tekran. Data streams from the unit were intermittent.
  - There was also a malfunction in the mass flow calibrator on the gas analyzers which was corrected during the last week in May.
- **June**
  - Malfunctioning of the Tekran unit persisted. Valid data collection was sporadic throughout the month.
  - The pump on the FRM sampler malfunctioned -the unit was replaced.
- **July**
  - A poster presentation of the SAM was presented at the NETL program review meeting in Pittsburgh PA.
  - Matt Landis from National Exposure Research Laboratory completed an on site audit of our installation and QA/QC procedures for the Tekran. Several steps in

our operating procedures including calibrations were modified based on suggestions by Mr. Landis.

August, September and October

- There was continuous data collection during this period. There was a good build up of data which included data from the Tekran.
- The monitoring site had many visitors including staffers with the Ohio Delegation. Data analysis was started, the preliminary results of which are briefly described below.

Summary of Mercury Data:

Atmospheric mercury data has been collected for approximately four months. The Tekran mercury vapor analyzer (2537A) is used in conjunction with a mercury speciation unit (1130) and a particulate mercury module (1135) to collect real-time semi-continuous comprehensive mercury data. The time series data for elemental, reactive gas and particulate mercury are presented in Figures 2, 3, and 4 respectively. While equipment problems and breakdowns remain common with this type of instrumentation, the majority of the data appears valid. The graphs use bi-hourly data, which has not yet been smoothed to remove noise.

The most obvious difference from this initial data set and other published data is the frequency and persistence of elevated mercury event impacts. For example, Edgerton et al. (2004) reported frequent RGM events on the order of 25 pg/m^3 at a rural site near Atlanta Georgia. In comparison the Athens SAM experiences frequent elevated mercury events exceeding 50 pg/m^3. Figure 5 shows an example of a typical elevated RGM mercury event. A detailed analysis of these elevated events is currently on-going and a summary of the analysis will be presented in subsequent reports.

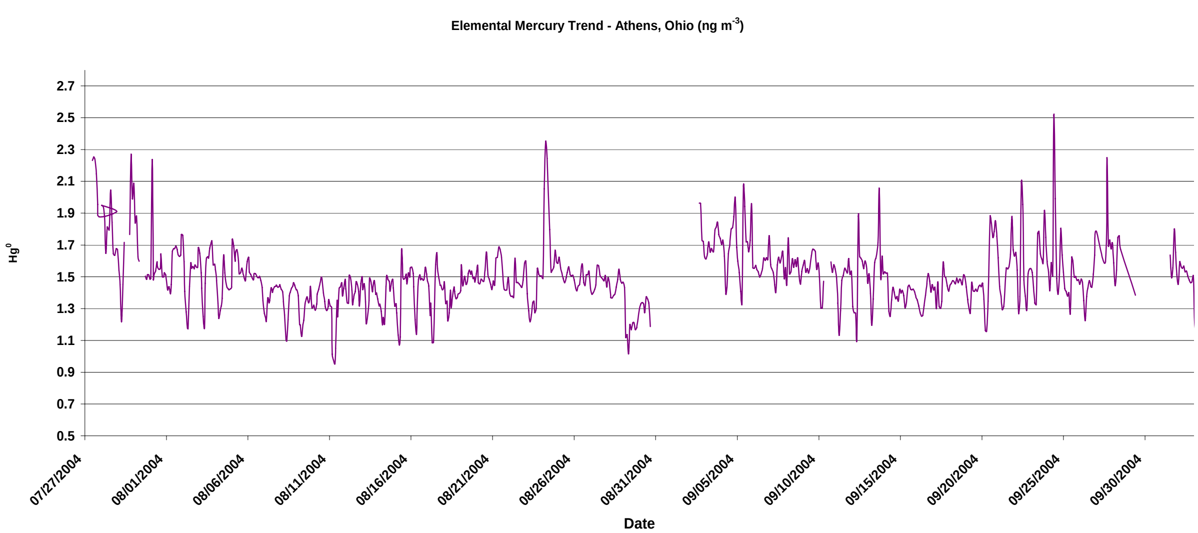


Figure 2. Time series of elemental mercury (Hg^0): July 27 to October 2, 2004

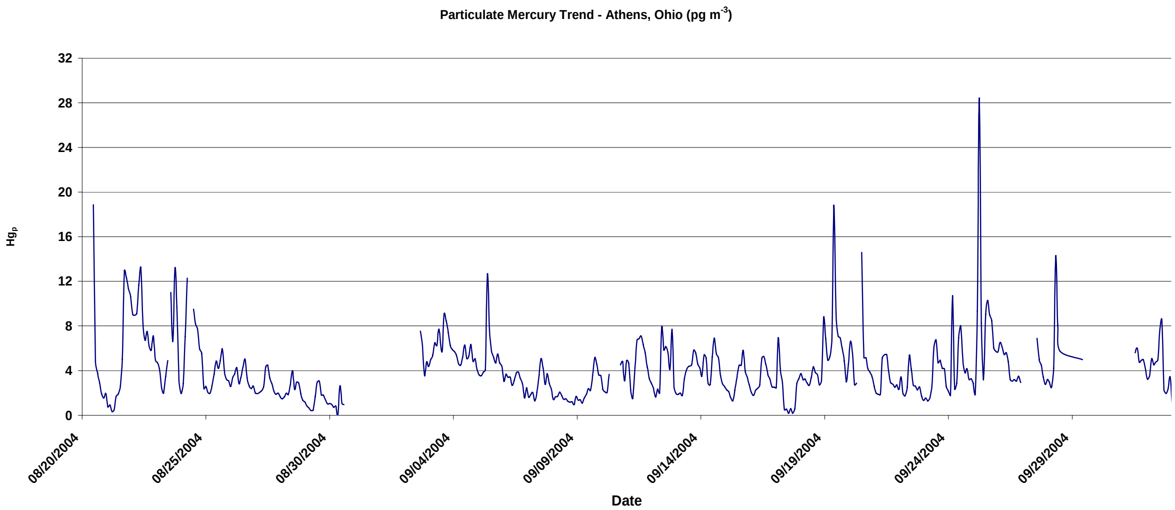


Figure 3**.** Time series of particulate mercury (Hg_p): August 20 to October 2, 2004

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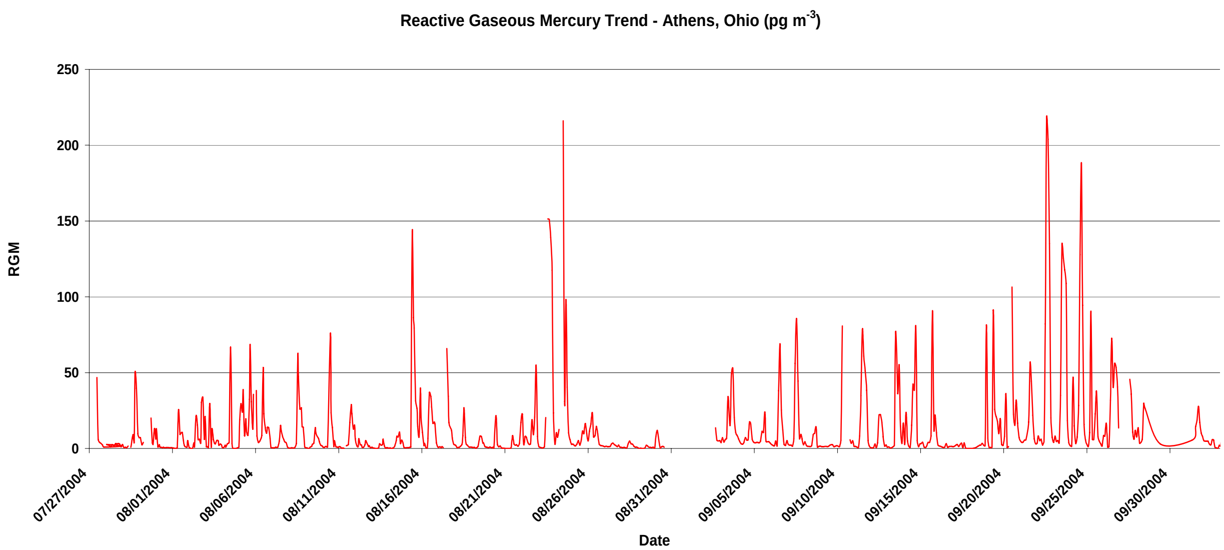

Figure 4. Time series of oxidized, or reactive gaseous mercury (RGM): July 27 to October 2, 2004.

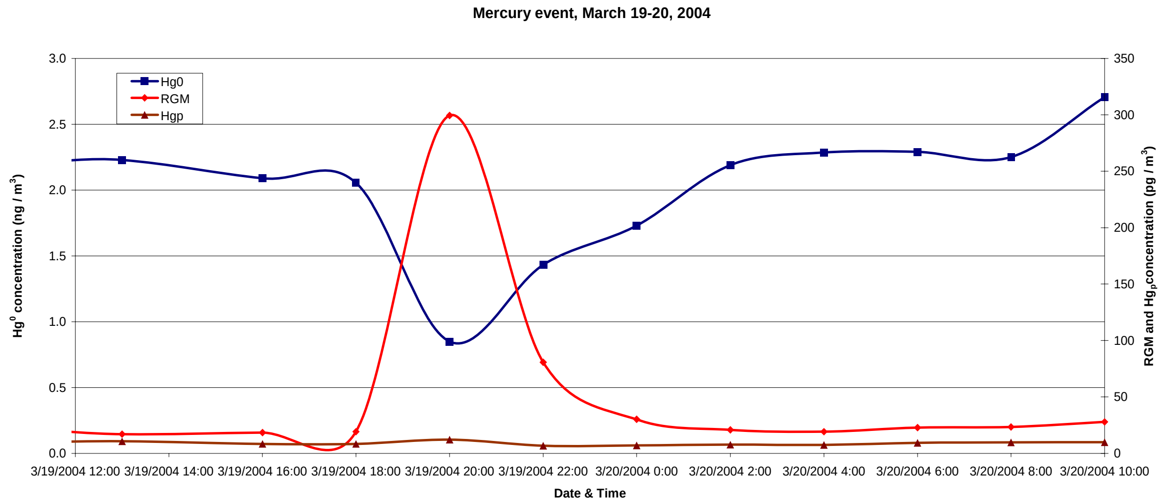

Figure 5. Elevated RGM mercury event: An RGM spike and with a corresponding Hg^0 depletion around 20:00 which is typical of elevated mercury events experienced at the Athens SAM.

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

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 from April 3, 2004 to October 2, 2004:

- Conducted annual simulations 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:
    - o 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 only saves the hourly values).

The preliminary results from the model simulation are currently being analyzed and will be presented in the next semi annual report.

Task 3 - Refine and Update Emission Inventories (EIs)

Advanced Technology Systems, Inc. (ATS) is enhancing the mercury and arsenic emission inventories.

Task 3 accomplishments from April 3, 2004 to October 2, 2004:

- 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.

Task 4 - Perform Short-Period Model Runs for Comparison with Field Data

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 will 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 set up and 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 will 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.

Task 4 accomplishments from April 3, 2004 to October 2, 2004:

- Work is underway to perform regional and urban modeling simulations for 36-, 12-, and 4-km-grid resolutions for the year 2004. 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 current parallel version of MM5 has been downloaded to the system. Observational meteorological data sets for 2004 are being acquired from the National Centers for Environmental Prediction (NCEP) to conduct 4DDA (four-dimensional data assimilation) as a part of MM5 simulations. The MM5 modeling simulations were conducted from January 1-January 11, 2004 in the nested mode (36km, 12km and 4km) using nudging four-dimensional data assimilation (4DDA) techniques towards observations. The results from the model evaluation will be presented in the next semi annual report.
- 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 results from this model evaluation are described below.
- 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.

Results and Discussions from CMAQ Simulations for July 2001.

The following specific milestone was completed during this reporting period:

Milestone: Calibration of a short-term atmospheric chemistry model which in this case is CMAQ using ambient monitoring data downwind of coal power plants. This task involved conducting short-term model simulations and comparison with field data. The time period selected was the summer of 2001 since hourly $PM_{2.5}$ data was available from the DOE-NETL sponsored super site at Pittsburgh PA during this period.

Results:
A CMAQ modeling simulation was performed for July 2001 for the contiguous US over a 36 km grid resolution. The vertical resolution consisted of 14 layers and the simulation used CB-IV gas-phase chemistry mechanism. CMAQ version 4 which incorporates aerosol module aero2 was used for this evaluation. Version 4 contains the CMAQ-Hg code that will be utilized during the sensitivity evaluations (Task 5).

There was a strong correlation between the model output and observational data for sulfate however, the model significantly under predicted nitrate concentrations. The under prediction of nitrate by CMAQ (version 4) is corroborated by Mebust et al. (2003). Mebust et al. attributed this deficiency in simulated nitrate concentrations to the annually averaged ammonia emission values provided in EPA's NEI inventory which does not reflect the seasonal variability in the emissions.

Figure 6 presents the time series plot of hourly observed particulate sulfate data from the DOE-NETL sponsored supersite at Pittsburgh in red and the corresponding model simulated data in blue. The plot shows a periodic variation in the measured sulfate concentration over a period of 21 days in July 2001. These periodic variations were captured by the model. A scatter plot of the modeled versus the observed is show in Figure 7. A strong correlation between the modeled and the observational data was experienced with an R^2 of 0.68. Some scatter is observed possibly due to biases in the sulfate deposition. A stronger correlation was obtained with the 24-hour mean observed sulfate data for the same time period with an R^2 of 0.76.

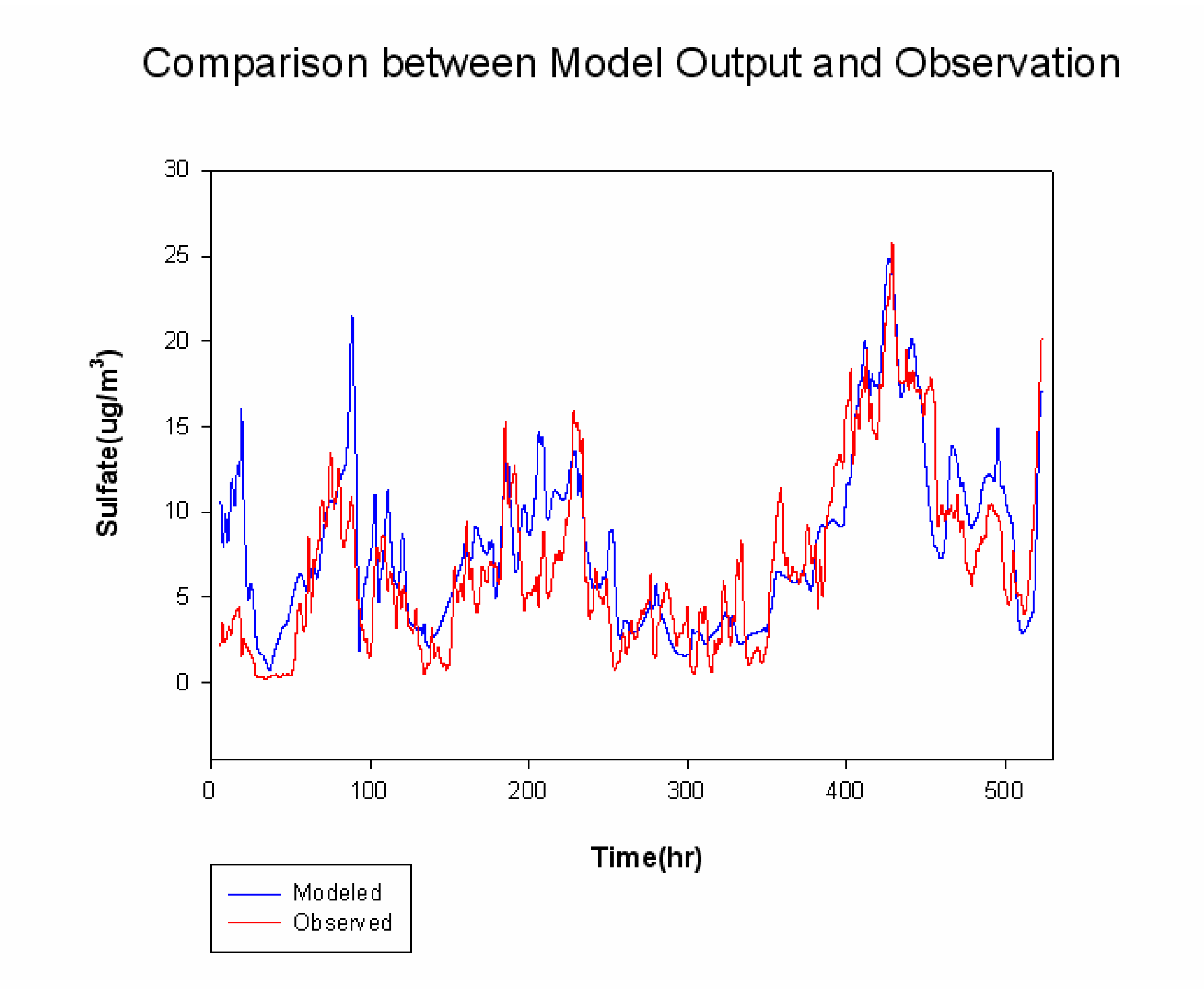

Figure 6. Comparison between model output and observation for particulate sulfate July 1- 22, 2001

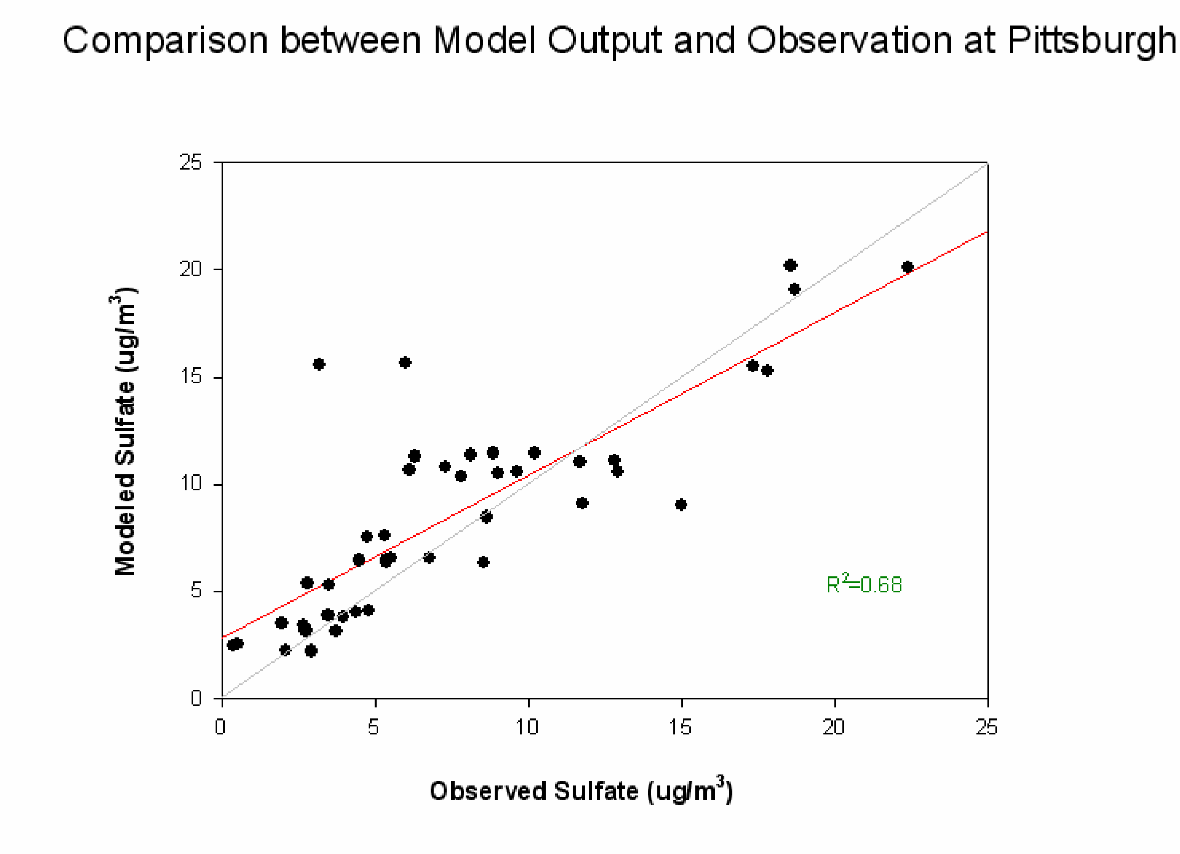

Figure 7. Regression plot for model output and observation for particulate sulfate

The model performance was further evaluated using statistical techniques. The mean fractional bias and error are considered the least biased and most useful among the statistical metrics. The mean fractional bias in case of sulfate was 30% for both hourly and mean values of sulfate. The mean fractional error was 50%. Statistically these values are within acceptable limits.

<u>Task 5 - Seasonal Scale Simulations</u>

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 from October 2, 2003 to April 30, 2004:

- The project staff has completed a one-year base case simulation for 1996. Work is underway to analyze the model output from this simulation. Further work on this task is slated for a later phase of the project.

Task 6 - Development of a Decision-Support Tool

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.

- The project staff has completed no work on this task, slated for a later phase of the project.

Task 7 - Project Management, Data Analysis, and Reporting

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.

III. SUMMARY OF RESULTS

The Cooperative Agreement began on April 3, 2004. A six month no cost extension was requested which will extend the project through December, 2005. During the third reporting period of this project (April 3, 2004 – October 2, 2004) Consol and ISEE continued the operation of the SAM site. The Tekran was malfunctioning during the first couple months of this reporting period but it has been extremely stable through the remainder of this reporting period. The site is acquiring a strong data set and preliminary analysis shows frequent elevated RGM events that will provided the platform for analysis of mercury speciation characteristics during transport and the evaluation of urban and point source emissions. A wind speed/wind direction sensor located at the top of an adjacent 400 foot communication tower was installed.

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. AER is currently analyzing the model output from the 1996 CMAQ run. The researchers at Ohio University have also conducted an evaluation of short-term model runs for July of 2001. The model output was evaluated against hourly measurements obtained from the DOE sponsored Pittsburgh Air Quality Study. Strong correlations were experienced for particulate sulfate concentrations. However the model under predicted the particulate nitrate concentrations.

ATS is currently upgrading 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.

IV. CONCLUSIONS

The initial phase of the project was delayed by approximately three months due to contract negotiations with the subcontractors. However, the monitoring efforts and the modeling efforts have been initiated and are proceeding as expected.

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