

**Quality Assurance Project Plan for the Air Quality Core**

EPA Clean Air Research Center

Southeastern Center for Air Pollution and Epidemiology

Emory University and Georgia Institute of Technology

Management Approvals:



10/5/11

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Ted Russell  
Co-Director and Air Quality Core Principal Investigator

Date



10/10/11

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Quality Assurance Advisor

Date

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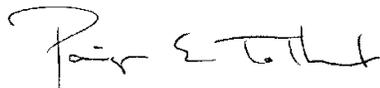
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10/6/11

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Paige Tolbert  
Co-Director

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10/8-2011

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## 1. Introduction

This QA Project Plan (QAPP) describes how planning, implementation, and assessment activities and management functions are coordinated to carry out the basic research and support functions involved in the “*Southeastern Center for Air Pollution and Epidemiology: Air Quality Core*”, funded by the US EPA through grant # RD83479901. This Quality Assurance Project Plan (QAPP) is intended to follow all guidelines and requirements of the EPA for a modeling project. To ensure compliance with EPA quality assurance requirements, we referred to quality guidance available from the EPA Office of Environmental Information (EPA 2001a, EPA 2001b, EPA 2002a, EPA 2002b, and EPA 2007) and prior QAPPs developed by Georgia Tech and approved by EPA.

We took the following steps and procedures to prepare this QAPP:

- Determine data quality objectives (DQOs) that are qualitative and quantitative statements of the quality of data needed to support specific decisions or regulatory actions.
- Define project-specific QA/QC requirements through detailed Statements of Work instructions. Identify the critical activities to be performed, those activities that are most prone to QA problems, and discuss the QA activities to be conducted during the validation phases of the project.
- Document Standard Operating Procedures (SOPs) for performing certain routine repetitive tasks. These tasks frequently involve such operations as data updates, software development and improvements, data collection, software manual development, presentation/visualization of results, and model applications.
- Specify procedures for assessing the quality of all deliverables generated and processed for accuracy, precision, completeness, comparability and representativeness.
- Include provisions for written requirements establishing and maintaining QA reporting or feedback channels to the management responsible to ensure that early and effective corrective action can be taken when data quality falls outside established data quality objectives or acceptance criteria. Also include provisions to keep management informed of the performance of all data collection efforts when corrective actions are necessary.

The overall objective of this QAPP is to ensure high-quality research results and that the deliverables of this project are of sufficient quality to support the intended use by EPA.

## 2. Project Organization

Two primary institutions are involved in this research: Georgia Tech (GIT) and Emory University, though other institutions play more minor roles in the Center and are not directly involved in the Air Quality Core. Georgia Tech’s expertise is in atmospheric model development and application. The lead staff involved in this project are Ph.D.’s with demonstrated expertise (e.g., via publications) in air quality modeling and data analysis.

Prof. Ted Russell (GIT) is the P.I., with overall responsibility for the supervising the Air Quality Core’s success. GIT will conduct the Weather Research and Forecasting (WRF) and

Community Multiscale Air Quality (CMAQ) simulations, conduct source apportionment using both EPA-supported and in-house developed methods, analyze air quality data, and store both observational and modeling data developed as part of this project. Included in the GIT team are Drs. Talat Odman, Yongtao Hu and James Mulholland. Dr. Yang Liu represents Emory University on this core. Dr. G. Zhu is the Quality Assurance manager at Georgia Tech.

### **3. Project and Air Quality Core Background**

In recognition of the extraordinary complexity of the relationships between atmospheric processes, human exposures to ambient pollution and associated biological responses, research is increasingly focusing its ambient air pollution health effects research agenda on consideration of cumulative effects of air pollutant mixtures. This represents an important evolution in emphasis, and will require fresh approaches to overcome challenges that pervade epidemiologic studies of real-world ambient air pollution. Issues impeding a full understanding of health effects of ambient air pollution from the existing body of literature are widely appreciated. Atmospheric processes driving transformation of the primary pollutants emitted from stationary and mobile sources lead to a dynamic ambient environment comprised of a multitude of agents with unique physical and chemical characteristics. Composition of the mixture thus varies over both time and space, and attempts to characterize the mixture are generally accompanied by measurement error that varies across the species of interest. Further, how humans move through the microenvironments and how their behaviors and activities alter their personal exposure to pollutants of ambient origin add further complexity. Finally, the physiological responses occur through a complex web of feedback loops on multiple time scales with interactions occurring among specific components and other individual-level factors such as other exposures and genetic constitution. Epidemiologic models focusing on single pollutants are prone to concerns about whether the pollutant is operating as a surrogate for an etiologic agent or group of agents. In the presence of differing levels of measurement error and/or unmeasured confounders, multi-pollutant epidemiologic models do not obviate this concern.

The Southeastern Center for Air Pollution and Epidemiology (SCAPE) is a multi-institutional, multi-disciplinary Center is proposed to address the critical issues noted above relating to the public health impacts of ambient air pollution. The overarching theme of the Center is a focus on characterizing ambient air pollution *mixtures* and elucidating their role in human health risks associated with air pollution. Novel measurements and modeling approaches will be applied in the context of a tiered multi-scale assessment of the health risks of mixtures characterized based on: 1) biological considerations (oxidants); 2) environmental management (sources); 3) evidence-based considerations (traffic emissions); 4) empirical assessment (data-based approach).

Four Research Projects will be supported by three Cores: an Administrative Core, an Air Quality Core and a Biostatistics Core. Project 1 will develop and deploy instrumentation to measure oxidants (including aerosol reactive oxygen species) and other species of interest to better understand their origins and atmospheric transformation and for use in characterizing mixtures for the three health studies. Project 2 will make direct use of these measurements to confirm associations with markers of oxidative stress in commuters. Projects 3 and 4 will use a combination of measurements and modeled air quality estimates in large population studies, with

Project 3 investigating questions regarding risks of *in utero* and early life exposures to air pollutant mixtures in two major new birth cohorts and Project 4 assessing underlying consistencies in morbidity associations across selected cities that have comprehensive daily air pollution characterization. The health projects include assessment of potentially sensitive and vulnerable subpopulations. The Air Quality Core will provide support functions to the primary projects and conduct additional research to develop new methods for more advanced analyses.

#### Air Quality Core

The Air Quality Core (AQC) has six functions identified to provide Center researchers the information and methods to comprehensively characterize air pollutant mixtures relevant to their projects. These functions are efficiently provided across the projects by a dedicated team, and take advantage of the pooled expertise of the AQC personnel and the extensive resources available to them. Function 1 is to collect and manage the wide range of air pollutant, meteorological and emissions data that is central to the individual projects. This data will include both observational and modeled data, including our on-going CMAQ-modeled forecast fields that can be used for planning field experiments. Function 2 is to develop a Mixtures Characterization Toolkit (or MC Toolkit) that center researchers can readily use to provide information on the pollutant mixtures, sources and atmospheric processing in their study areas. MC Toolkit will include analyzed data, regression models, receptor-based source apportionment models, source-based air quality models, including CMAQ and a microscale dispersion model. These models will be extended using data from Projects 1 and 2. As the developers, AQC will support center researchers in applying MC Toolkit (Function 3). AQC personnel have developed significant expertise in extending and applying CMAQ, and an initial effort will be to conduct an annual CMAQ simulation, with increased resolution over the project areas, to provide each of the project teams a spatially, chemically and temporally comprehensive characterization of pollutants and sources (Function 4). Satellites are providing an increasing wealth of air quality-relevant information which can be further used to indicate the spatial and temporal evolution of pollutants, and for comparison with model results. Satellite retrievals will be used to provide additional information on various pollutants and the impact of forest fires in the area, which is of increasing concern as controlled burns are used with increasing frequency (Function 5). Finally, Function 6 extends our prior work on assessing exposure misclassification, using the unique data and models available from the center activities to consider population exposures within and across scales.

#### 4. Core Functions

The AQC will have six functions (described below) in support of the four research projects and other cores within the Center. In addition to these functions, the AQC team will assist in the preparation of reports and journal publications resulting from Center activities. In the following sections, the AQC is described in terms of its personnel and structure, its approach, and its interactions with Center projects and core activities.

*Function 1. Atmospheric data collection and management. Atmospheric data from Projects 1 and 2, along with routine, satellite and other special study observations will be collected for general use by Center projects and outside and for integrated analyses by AQC researchers as outlined in Functions 2-6. Support of Projects 1, 2, 3, 4.*

*Function 2. Development of the MC Toolkit to support Center projects. MC Toolkit will include processed and analyzed atmospheric data, analysis methods and air quality models for use by project teams. As part of the toolkit development, technique capabilities will be extended with particular focus on unique trace components to make use of the comprehensive ambient measurements. Components of MC Toolkit will*

*include:*

- *Data analysis products, descriptive assessments of observations, statistical analysis of individual pollutants, pollutant and meteorological data visualizations; in-situ, satellite and model products*
  - *Receptor-oriented data analysis and source apportionment methods, including regression approaches and receptor source apportionment (CMB, PMF, UNMIX)*
  - *Source-oriented air quality models, including CMAQ chemical transport model and Mobile Matrix-CALINE Grid*
  - *Hybrid receptor and source-oriented source apportionment model providing mixture characterization*
- Support of all projects.*

*Function 3. Support of project teams using MC Toolkit for data analysis, model applications and interpretation of results. Support of Projects 2, 3, 4.*

*Function 4. Application of the extended Models 3/CMAQ to provide a comprehensive characterization of pollutant concentrations, sources and variations. CMAQ will be applied over a domain covering the continental US using finer spatial resolution over project study areas. The large scale application will provide an assessment of how air pollutant mixtures in the study areas compare to other regions. Finer scale nesting within the project areas will be done to inform project personnel as to the spatial, temporal and chemical variations that are not directly available from observations. Products of this Function will be added to MC Toolkit in support of Projects 1, 2, 3, 4.*

*Function 5. Integration of satellite remote sensing into health studies and air pollutant mixture characterization. Satellite retrieved aerosol optical and microphysical properties and biomass burning parameters will be used with land use data to characterize the spatial patterns of particulate properties as well as the spatial impacts of wildfires and prescribed burns. Processed data will be added to the MC Toolkit. Support of Project 3.*

*Function 6. Assessment of exposure misclassification across scales and source regions. Included in this task will be the use of detailed information of pollutant concentrations at multiple temporal and spatial scales from Project 1 to assess exposure error when considering populations within and across scales. Support of Projects 3, 4.*

## **5. Quality Objectives and Criteria for Model Inputs/Outputs**

The success of this effort will be measured, first by our ability to provide the type information to the various project teams at a quality level that meets or exceeds their needs. Second, our success will be gauged by our ability to advance the tools being used by the community (scientific and policy-making). Finally, success will also be measured by the acceptance of manuscripts submitted for publication and the quality of the graduate student's theses.

Three project elements are applicable to this support core: acquisition, maintenance and analysis of air quality data, the use of existing/ secondary data, and development or refinement of models.

Acquisition, maintenance and analysis of data: We will collect air quality (and related) data, including pollutant concentrations, emissions, meteorological variables and land uses, that will be used by the four project teams. This data will be analyzed by core personnel for integrity using various graphical methods. The data will be maintained on the SCAPE project website. Various data analysis approaches will be used to assess correlations to identify characteristics of potential interest.

Use of existing secondary data: We will review secondary/existing data collected as part of the various regional and national emission inventory efforts (EPA's NEI, RPO's EI for regional SIP efforts). To judge the quality of secondary data, we will apply the data quality ranking for this data,

and apply technical judgment to this secondary data, including an assessment of how and by whom the secondary data was gathered. The primary concerns of Georgia Tech are that the data are fully documented, and translated properly into the database with required units properly calculated, and that they are accurate representation of the information provided in the reference source.

**Development and Refinement of Models:** We will address project needs primarily computationally, and thus quality of the study is assured primarily through model testing, using quality-assured data, model performance analysis conducted using observed data, model inter comparisons, code-checking, peer review, exchange of results and cross laboratory and platform comparison of identical calculations. For example, we generally assure that our model performs at least as well as the EPA guidelines for ozone modeling, and we follow the draft guidelines for PM modeling. This includes diagnostic simulations (e.g., impacts of boundary conditions, initial conditions, zero emissions, etc.). Model evaluation is planned for this study, though WRF, CMAQ, Chemical Mass Balance (CMB) and Positive Matrix Factorization (PMF) are extensively used and have been peer-reviewed. Data reduction will primarily be done through developing of overall statistical measures characterizing the myriad of results available from models, and we will also use visualization (generally using PAVE©, developed by MCNC). Statistical analyses are typically done using Excel © and R.

## **6. Documentation and Records**

Use of existing/secondary data will be fully documented with data's original documentation archived. We will provide additional documentation when necessary to address the issue of particular data points that seem less reliable than others.

Results and codes will be documented and will be backed-up on streaming media or DVD, as well as on our RAID's and disk backup library. In addition, we will use revision control utilities to maintain and archive codes.

Results of the study will be submitted for peer review and publication. AQC analysis will also be the basis of two students' theses, which will be reviewed by no less than five individuals. In addition, the results and codes used will be made available via the web site <http://scape.ce.gatech.edu>. We strongly support making available all codes, model inputs and results for use by others, both to extend our work, but also to check our work.

## **7. Data Acquisition and Model Calibration Evaluation**

The types of data to be acquired and maintained at Georgia Tech include air quality, emissions, and meteorological variables. Air quality data will be acquired both from other SCAPE project work (particularly Projects 1 and 2), and from outside. Outside data sources will include EPA (e.g., using the Air Quality System (AQS) data base), states (if the state-collected data is not stored by EPA), individuals operating special sites (e.g., SEARCH and the St. Louis and Pittsburgh Supersite P.I.'s) and satellite retrieval products (e.g., from NASA and NOAA).

Emissions inventories are developed from standard data bases, and are quality-checked at GIT. The foundation of the historical inventory being used has been checked as part of the VISTAS project by the Georgia DNR, ourselves and others. After emissions processing, details (e.g., county-wide totals) are compared to prior analyses to monitor the possible introduction of errors in

that process. Model outputs have, in the past, and will be checked against other groups simulating the same period to identify anomalous behavior.

A major component of this project is the evaluation of the downscaled fields, and the air quality model results resulting from the use of those fields. This will be done by comparing model results to observations, results from our past climate project, and comparison to other groups. This will involve developing statistical distributions of key meteorological and air quality model outputs, and comparing those distributions against the corresponding distributions of the observations. Meteorological model results will be compared against National Center for Environmental Prediction data, while air quality results will be compared against data from the routine monitoring networks, and stored by EPA (e.g., AQS and STN data). This data has undergone its own set of QA/QC, and is traditionally used for model evaluation. In our handling of the data, we will perform visual and statistical checks to assure that it is being handled properly. Our past model evaluations are available in the literature, including our use of statistical distributions in model evaluation.

A major focus of the AQC is to provide improved source impacts to the project teams (particularly Projects 2-4). These source impacts will be derived using a number of methods, and their consistency will be investigated, however, there is no way to actually measure source impacts directly. Thus, one aspect of this research area is to develop methods to better evaluate the accuracy of the various source apportionment methods. The methods developed for assessing accuracy will be submitted for publication.

## **8. Hardware/Software Configuration and Data Management Plan**

Computations will be conducted at GIT. The air quality group has approximately 20 single and five multiprocessor Sun and Linux workstations/clusters and an SGI 8-processor workstation on which they apply the Sparse Matrix Operating Kernel for Emissions (SMOKE), WRF and CMAQ modeling, along with over 25 terabytes of online storage and streaming media back up. We have recently ordered a 64-core cluster along with an additional 10 TB of storage. If, for some reason, additional computing resources are required, as a professor at GIT, Dr. Russell can get access to the GIT computer facilities that include SGI multiprocessor machines and Linux clusters. Facilities are behind strong firewall and are protected for data security.

The WRF/SMOKE/CMAQ system represents the state-of-the-science in regional air quality modeling, and is chosen for performing the air quality simulations. WRF, SMOKE and CMAQ are relatively well known and extensively documented models. In addition to its scientific foundation, the widening community of users makes this system attractive for use. The version of CMAQ (v4.7) used will have SAPRC-99 and DDM-3D, the Decoupled, Direct Method in Three Dimensions, a method to directly and efficiently calculate the sensitivity of model outputs to model inputs. The most recent version of CMAQ has added additional chemistry to deal with a low bias in OC (organic carbon), and additional routes (e.g., via water-soluble organic compound (WSOC) formation and partitioning) will be added by us.

The GIT computer systems are professionally managed, facilitating data management activities. Disk arrays are routinely backed up. However, the sheer volume of data that will be produced by the atmospheric modeling systems lead to significant data management issues, though

we are well acquainted with the needs from prior modeling projects. In addition to having over 25 TB (soon to be 35 TB) of on-line data storage, the SCAPE researchers maintains a library of off-line back-up disks, organized by project and date. Transmission of large data sets between institutions is typically accomplished by mailing external disks containing the data (which is backed up and verified before sending).

Based on our past projects of similar magnitude, we expect that approximately 20 terabytes of computer output will be generated in conducting this project, making data management and dissemination planning integral to both the successful conduct of the project, as well as ensuring its legacy and use by others. Georgia Tech will provide public access to all relevant and significant datasets generated in this project, though given the large amounts of data generated, not all data would be stored on the servers. Georgia Tech will be responsible for maintaining all data with major data products stored on websites available to Emory and Georgia Tech via a password protected link. The web site is hosted on the GIT CE web server which is professionally managed by trained personnel. Abbreviated final air quality model outputs and air quality data that are used in publications would be stored on a non-password protected portion of the site. Downloading data from these websites would be free. Complete data sets, which often comprise many TB of data and thus are not amenable to being stored on-line, will be stored off line on disks.

The size of many of the undigested WRF and CMAQ model inputs and outputs make internet transmission prohibitive, so only subsets of model outputs (e.g., ground-level ozone and PM species concentration fields and sensitivities for each of the simulations), along with the codes used to generate those results, would be made available on the SCAPE web site (<http://SCAPE.ce.gatech.edu/>). The site would also describe how to obtain complete model inputs and outputs (see below). This web site has been created for this project, and the School of Civil and Environmental Engineering at Georgia Tech provides on-going support for professors to maintain such websites. In addition to providing descriptions of group activities and personnel, this site has been used for data storage and transmitting data to collaborators. As we do with all our data sets, we will provide documentation of the data sets itself, and guidance in their use. Given their size, all raw meteorological and air quality model inputs, outputs, along with the codes used to generate them, will be archived on additional off-line hard drives in the SCAPE storage disk library. Funds have been allocated to purchase storage disks.

We are committed to providing our data files and codes for use by others, both to extend our work and to independently verify our calculations. For example, in the recently completed STAR grant project, our results were provided to the University of Illinois for compilation and comparison to other modeling results. To facilitate such activities, WRF and CMAQ input and output data sets will be stored in our disk library in a form for direct use by others in similar simulations. CMAQ outputs will be stored in netcdf for compact transmittal and ready use. As done in our prior projects, for requests requiring very extensive amounts of data, we will send external hard drives with the data at cost. Computer codes, including the WRF and CMAQ versions used, will be stored and made available along with the model results. Given past experience, we expect that this will be the primary mode of data transmission, and our ability to successfully transmit data in this mode both during and after project termination has been demonstrated.

## **9. Assessment and Oversight**

The Principal Investigator and other AQC staff frequently present project work to EPA staff, external reviewers, and internal researchers. These presentations provide timely reviews of the project design, implementation, and interpretation of the project results. The assessments of overall project quality are provided from a number of different sources. Internal reviews of selected project components are periodically performed by the Principal Investigator. The results of this and other routine (e.g., QA/QC checks) and special reviews of project data quality will be documented in annual reports.

The quality of the project data will be maintained not only through the development and use of data quality objectives (DQOs), which place numerical limits on the quality control indicators, but also through the use of subjective science quality objectives. Science quality objectives are used to provide evaluations of the quality of the research project and goals of the study. Evaluations of all research activities by internal and external peer review will assure that the methodology, experimental processes, conclusions and recommendations provided by this project are scientifically sound.

Assessments of the quality of the products generated on this project will be made by:

- Conducting internal performance reviews of the critical components of the model setup and data processing systems. Where applicable, adherence to SOPs will be evaluated. The results of these reviews will contain any suggested corrective actions, and be appended to the reports generated in this project.
- Independent peer reviews of thesis materials, reports, and papers resulting from this project. The U.S. EPA project officer provides external review of all reports and plays a role in the project and to review research progress and plans for future project tasks.

Routine QA/QC checks for this project's modeling efforts will be:

Air Quality Data:

- Examine and compare data values with other locations at the same time, and the same location at other times.
- Plot data to identify outliers.
- Compare data to model results when possible.
- Conduct simple data analysis, including correlations with other, related data.

Emissions Data:

- Examine and compare data values, and weigh the facts against expert knowledge of the subject to reach a conclusion about the validity of the data. This process is also known as "engineering judgment" or "expert judgment."
- Use statistical tools and measures to evaluate emissions data sets. Commonly used statistical approaches used to QA emissions data (e.g., emission estimates, emission inventories) include:
  - Descriptive statistics (mean, standard deviation, frequency distributions, etc.) are used for data presentation and to facilitate peer review;

- Statistical procedures are used to detect outliers and to verify that data are reasonable; and
- Statistical tests, such as t-tests or similar analyses, are used for comparability checks (e.g., to compare two or more data sets), for data validation, or for evaluating the relationships between parameters.

#### Emissions Modeling:

- Although the SMOKE system will screen out errors in input data, some additional input error checking algorithms are used to screen the data and identify potential emission input errors. Additionally, EPA has issued QA and data augmentation guidance for stationary point sources that can be used to identify and augment any outlying stacks.
- SMOKE provides various cautionary or warning messages during the emissions processing. These messages are redirected to output log files which are then reviewed for serious error messages. An archive of the log files is maintained so that the error messages can be reviewed at a later date if necessary.
- The QA functions built into the SMOKE system are utilized to provide summaries of processed emissions as daily totals according to species, source category and county and state boundaries. These summaries will then be compared with summary data prepared for the pre-processed emissions, e.g., state and county totals for emissions from the augmented emissions data.

#### Model-Ready Emission Inputs

- The goal of the post-processed emissions summary QA is to detect possible errors in the final, model-ready binary emissions files by preparing summary plots that characterize spatial and temporal patterns in the emissions data. This step is designed to catch errors that may be missed in the internal emission model QA procedures. We will produce the following graphics for QA checks:
  - Spatial Summaries: Sum the emissions for all layers and for all 24 hours and prepare plots showing the daily total emissions spatial distribution. The objective of this step is to identify errors in spatial distribution of emissions.
  - Vertical Profiles: For point sources the emissions total for each layer are summed and plotted to show the vertical distribution of emissions. These plots show the emissions on the x-axis for each model layer on the y-axis. The objective of this step is to identify possible errors in vertical distribution of emissions.
  - Short Term Temporal Summary: The total domain emissions for each hour are accumulated and time series plots prepared that display the diurnal variation in total hourly emissions. The objective of this step is to identify errors in temporal profiles.
  - Long Term Temporal Summary: The total domain emissions for each day will be accumulated and displayed as time series plots that show the daily total emissions across the domain as a function of time. The objective of this step is to identify particular days for which emissions appear to be inconsistent with other days for no obvious reason (e.g., not a weekend) and compare against the general trend.

- Control Strategy Spatial Displays: Spatial summary plots of the daily total emissions differences between base and different emissions scenarios will be generated. These plots can be used to identify issues in scenario emissions.

#### Meteorological Model Output:

- Create horizontal and vertical plots of temperature, pressure, precipitation, modeled flow patterns, PBL heights, etc. to assess whether the air quality model-ready meteorological data fields are reasonable; and
- Evaluate the modeled meteorology to assess whether the downscaling of WRF keeps the main patterns generated by the global model such as Model E outputs.

#### Chemical Transport Air Quality Modeling:

- Verification that correct configuration and science options are used in compiling and running each component of the modeling system, where these components include the meteorology pre-processor, initial/boundary conditions processors, photolysis rate calculators, chemistry-transport model (CTM), and any other preprocessor used to prepare data for the CTM.
- Verification that correct input data sets are used when running each model.
- Evaluation of model results to verify that the output is reasonable and consistent with general expectations.
- Processing of ambient monitoring data for use in the model performance evaluation.
- Evaluation of the air quality model results against observations.
- Backup and archiving of critical model input data.

#### Receptor-Based Air Quality Modeling:

- Verification that correct configuration and options are used running both the EPA-provided CBM and PMF models.
- Verification that correct input data sets are used when running each model.
- Evaluation of model results to verify that the output is reasonable and consistent with general expectations.
- Processing of ambient monitoring data for use in the model performance evaluation.
- Evaluation of the air quality model results against observations.
- Backup and archiving of critical model input data.

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