

APPENDIX B | UNCERTAINTY ANALYSIS OF THE INTEGRATED AIR
QUALITY MODELING SYSTEM

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APPENDIX B: UNCERTAINTY ANALYSIS OF THE INTEGRATED AIR QUALITY MODELING SYSTEM FOR USE IN THE U.S. ENVIRONMENTAL PROTECTION AGENCY'S SECTION 812 SECOND PROSPECTIVE ANALYSIS

Under Section 812 of the Clean Air Act Amendments (CAAA), the U.S. Environmental Protection Agency (EPA) is requested to periodically conduct and submit to Congress a report on economic benefits and costs of all provisions of the Act and its Amendments. The EPA delivered the first of these reports, a retrospective analysis covering provisions of the original Clean Air Act during the period 1970-1990, in 1997, and the second report, a prospective analysis covering provisions of the CAAA during the period 1990-2010, in 1999.

In September 2004, Sonoma Technology, Inc. (STI) completed an initial literature review that summarized much of the existing uncertainty literature and assessed the possible application of existing approaches to the Second Prospective Analysis for estimating the uncertainties in the integrated air quality modeling system (IAQMS), which includes the emissions, meteorological, and air quality models.¹

This appendix reflects updates to that prior work that were completed in October 2008, and includes three sections. First, this appendix provides an updated literature review of uncertainties in IAQMSs and methods for quantifying them (Section 1). Second, this appendix provides a summary evaluation of the overall reliability of IAQMSs (Section 2). Third, this appendix includes a discussion of the IAQMS used in the Second Prospective Analysis and a draft table that summarizes key uncertainties in the IAQMS, potential sources of error, potential biases for the net benefits estimate, and the likely significance relative to key uncertainties in net benefit estimate (Section 3). References cited throughout this document are provided at the end of the appendix.

UNCERTAINTIES IN THE IAQMS*Sources of Uncertainty*

Uncertainty in estimated values for future air quality arises from at least three sources: (1) inherent or stochastic variability in the observations; (2) errors in model physics and chemistry assumptions; and (3) errors caused by uncertainties in model input variables. For prospective analyses, we need to focus on uncertainty in the context of model response to future-year emissions. For example, an air quality model (AQM) may be very sensitive to a particular input without affecting its response to emission changes. Alternatively, an AQM may show little sensitivity to an input under current conditions

¹ See September 30, 2004 memorandum to Nona Smoke and James DeMocker, EPA/OAR/OPAR, from Neil Wheeler and Kiren Baum, Sonoma Technology, Inc., "Response to SAB Council Comments on the May 2003 Draft Analytical Plan for the Section 812 Second Prospective - Options for Uncertainty Analysis for Emissions and Air Quality Analyses".

(e.g., boundary conditions) but become increasingly sensitive to that input in future years as anthropogenic emissions are reduced.

Measurement Uncertainty

While measurement uncertainty is less important when using relative reduction factors (RRFs) and linear cost-response functions, it can affect the ability to evaluate model performance and gain confidence that a model is getting the right answer for the right reason. For gases, instruments can be calibrated using gases of known concentrations, and the uncertainty in the measurement is reasonably well known. However, this is not the case for PM. Uncertainties in PM mass and speciation can be significant, which limits our ability to critically evaluate model performance and reduce uncertainty in model simulations.

Hogrefe et al. (2000) developed an approach to gain insight into the distribution of future air quality predictions attributable to variability in currently observed air quality at a given location. The procedure is to fit a theoretical statistical distribution to the tail of a set of daily observations at a monitoring site (e.g., over a three-year period) and compute a design value consistent with the form of the National Ambient Air Quality Standards (NAAQS). The next step is to perform a bootstrapping operation several hundred times to obtain different sets of air quality data. For each instance, a design value is determined from the resulting data. The result is a distribution of current design values, which can be translated into a distribution of future air quality estimates using the RRF approach recommended in EPA guidance. While work so far has focused on the 1-hr and 8-hr NAAQS for ozone, it may be possible to apply the methodology to PM-related applications.

Model Uncertainty

Emissions, meteorological, and air quality models are mathematical representations of the physical world, and as such, have inherent uncertainties associated with their formulation, assumptions, and implementation. Some of the uncertainties are due to the limitations of our scientific knowledge. Other uncertainties are a result of simplifications or approximations needed to make the model practical. At the present time, we do not see a way to completely quantify uncertainty caused by inherent limitations in a model. However, methods and a body of research are available to help us understand the importance of uncertainty in individual model components. We can also reduce uncertainty by using models whose scientific basis is fully and satisfactorily explained in its accompanying documentation.

In some cases, it is necessary to use a simplified “engineering” or “reduced-form” version of a model. Uncertainty inherent in such results may be reduced if it has been shown that the engineering and more complete versions of a model produce similar results under the conditions that are of greatest interest for a particular application.

Input Uncertainty

The best-formulated and least uncertain models are only as good as their inputs. Model input uncertainty has been explored extensively in past decades and has driven research to improve these model inputs. In some cases, these inputs are based on measurements, which may be available only at limited temporal or spatial resolutions. In other cases, the input for one model may be the output of another model (i.e., the use of a mobile source emissions model to provide input to an AQM).

Methods for Assessing the Effects of Uncertainty

Sensitivity analysis is the most widely used method for assessing the effects of uncertainty on future-year air quality outcomes. Process analysis has been used in more recent AQM applications to identify those processes in the AQM that contribute the most to predicted pollutant concentrations and, thus, may be most affected by uncertainty. These methods and their use are discussed in greater detail below.

Sensitivity Analysis

The response of AQM predictions to changes of input parameters or model options can provide valuable information about uncertainties in model predictions. Such information can be obtained by sensitivity analysis, the systematic calculation of sensitivity coefficients, to quantitatively measure these dependencies. Basic sensitivity analysis may involve perturbing input parameters or model options one at a time or in combinations.

Beck et al. (1997) provide an overview of evaluations and uncertainties of environmental models, with emphasis on water quality models. They stress the need to specify a hypothesis or question to be answered by the model, and describe three alternatives to basic sensitivity analysis: (1) brute-force MC uncertainty analysis; (2) response surface evaluation; and (3) first-order error analysis, which is sometimes called sensitivity or “small perturbation” analysis. Each technique is discussed below.

Basic Sensitivity Analysis

Because of its ease of use and interpretation, there exist many examples of basic sensitivity analysis applied to AQMs. For example, Seigneur et al. (1981) estimated the sensitivities of an urban model to variations in input data. Winner et al. (1995) and Dabdub et al. (1999) showed that ozone predictions are especially sensitive to the inflow boundary conditions in Los Angeles and the San Joaquin Valley, respectively. Hass et al. (1997) carried out a sensitivity study of four European long-range transport and dispersion models, finding factors of 2 to 3 differences in the sensitivities of the different models to variations in emissions. Our review of these sensitivity studies suggests that the results are applicable only to a narrow range of conditions associated with the specific scenario. Because photochemical processes are often non-linear, the magnitude and even the sign of the sensitivity coefficients may vary as the scenario varies.

While meteorological parameters are undoubtedly important in photochemical grid models, it is not easy to decide how to account for variations in meteorology, especially

wind speed and direction. The problem is that it is necessary for the wind field to always satisfy mass-continuity, so that it is not correct to simply randomly vary the winds in each grid square of the model. Photochemical grid models make use of meteorological preprocessors, which may adjust the wind fields so they are mass-consistent. Hanna et al. (1998) avoided this problem by assuming that the perturbations in wind speed and direction applied uniformly across all grid squares. Schere and Coates (1992) suggested a more elegant (and time-consuming) method of accounting for uncertainties or variations in winds. Bergin et al. (1999) attacked the problem by generating a small number of alternate wind fields based on systematically “withdrawing” data from the meteorological preprocessor. This method is a useful first estimate but will underestimate the total uncertainty because of the limited number of runs and the failure to account for the full range of wind uncertainty.

Meteorologists have accounted for variability in weather forecasts by applying the “ensemble” method in which several forecast models (i.e., an ensemble) are run for the same scenario, and the best-guess forecast is assumed to be given by the mean of the several forecasts. These methods have been applied to air quality models by Straume et al. (1998), who showed that the ensemble method produced improved forecasts of tracer concentrations for the long-range ETEX tracer experiment in Europe. It is implied that the uncertainty would be given by the variability of the forecasts. These methods have also been extended to regulatory air quality modeling by using and evaluating alternative AQMs. For example, Ozone Transport Assessment Group (1997) modeling used multiple meteorological models (SAIMM and RAMS) and multiple AQMs (UAM-V and CAMx) for some episodes. However, it is clear that the full range of possible input conditions can not be covered by these ensemble methods.

The EPA guidance documents on attainment demonstrations (U.S. Environmental Protection Agency, 1999, 2001) identify three sensitivity tests that may be useful for assessing uncertainty in AQM predictions. The first of these, which has been proposed by Reynolds et al., (1996), is to prepare “alternative base-case” emission estimates, reflecting reasonable alternative assumptions about current emissions that lead to comparable or better model performance. A second test is to assume alternative (reasonable) growth assumptions. This could reflect using differing growth rates or placement of new sources in different, equally probable locations. Combinations of these first two tests are also possible. A third test involves simulating a future-year case with an alternative grid resolution or with different (reasonable) meteorological assumptions. For example, due to resource constraints, it might be necessary to perform modeling using a grid with 36-km grid cells (horizontal dimension). Differences in projected air quality obtained with a grid having 12-km or 4-km cells could then be evaluated.

The EPA guidance documents on modeling for attainment demonstrations were influenced by earlier guidance developed at the California Air Resources Board (CARB), which specifically addressed uncertainty (DaMassa, 1992). CARB applied this guidance in a series of uncertainty analyses to support the development of California’s State Implementation Plans (SIPs). This program included analyses of uncertainty associated with future-year boundary conditions (Wagner and Wheeler, 1988), meteorology

(Wagner and Wheeler, 1989; Wheeler, 1992), emission inventory bias (Wagner et al., 1992), horizontal advection solvers (Odman et al., 1996), chemical mechanisms (Whitten and Killus, 1998), and photolysis rates (Vuilleumier et al., 2000).

Monte Carlo Uncertainty Analysis

Monte Carlo (MC) methods are the most widely used means for uncertainty analysis. These methods involve random sampling from the distribution of inputs and successive model runs until a statistically significant distribution of outputs is obtained. There has been a rapid growth in the use of MC uncertainty analysis with photochemical AQMs in recent years. This “brute-force” method is computer-intensive because it requires 50 to 100 or more model runs for each base-year and future emission scenario. However, because of the exponential growth of computer speed and storage, it is now possible to carry out MC runs with a complex photochemical grid model applied to large domain. This method has been widely used in other environmental fields (e.g., water pollution modeling), as described in the reviews by International Atomic Energy Agency (IAEA) (1989), National Council on Radiation Protection and Measurements (NCRP) (1996), and Beck et al. (1997).

One of the first applications of MC uncertainty analysis to photochemistry was the study of relationships between stratospheric ozone and chlorine reported by Solarski et al. (1978). Alcamo and Bartnicki (1987) used MC methods to study the uncertainties in sulfur deposition predicted by the EMEF-W model in Europe. They found that it is more important to specify the width (i.e., the standard deviation) rather than the shape of the probability density function of the input variables. Irwin et al. (1987) performed an MC uncertainty analysis to estimate error bounds from the output of a Gaussian dispersion model. Uncertainties in wind speed, standard deviation of vertical and lateral wind direction fluctuations, and plume rise were propagated through the modeling system. It was found that the error bounds for the maximum concentration could be double that of the error bounds for the input parameters. This is one of the earlier papers on using uncertainty analysis on a dispersion model. Gao et al. (1996) applied MC uncertainty analysis to the chemical rate parameters. Deuel et al. (1998) studied the uncertainties of the UAM-V model using MC methods; however, the uncertainty ranges that they assumed for the input variables (vertical resolution, vertical diffusivity, plume-in-grid method, land-use, chemical reaction rates, and emissions) were a third or less than those recommended by the experts in the studies by Hanna et al. (1998, 2001). Bergin et al. (1999) applied MC methods with Latin Hypercube Sampling (LHS) to a Lagrangian photochemical AQM (i.e., not a grid model) in Southern California. They accounted for meteorological variability by using several solutions of a mass-consistent wind model, run with random data-withholding assumptions.

Frey (1992) discusses the decision process followed in applications of MC uncertainty analysis, stressing the importance of good estimates of input data uncertainties. Conover (1971) provides guidance concerning the computation of statistical tolerance limits from a simple random sample. Bergin et al. (1999) discuss the use of LHS, which they believe provides a better coverage of the data distribution than Simple Random Sampling (SRS).

However, the advantage of LHS comes with a price—only with SRS can the confidence in the results be interpreted through statistical tolerance limits.

From a practical standpoint, Hanna et al. (2001) demonstrated that MC methods could be applied to larger photochemical modeling studies (i.e., OTAG) by performing 100 simulations each for a base-case and three emission reduction scenarios. Hanna and Davis (2002) evaluated the UAM-V photochemical grid model by examining probability density functions of the variations in modeled ozone concentrations. The probability density functions are generated from 100 MC uncertainty simulations based on uncertainties in model input variables.

Houyoux et al. (2003) simplified the use of AQMs for assessing emission inventory uncertainties by generating multiple realizations of model-ready emissions with the Sparse Matrix Operator Kernel Emissions (SMOKE) processing system (Coats and Houyoux, 1996) by modifying SMOKE to accept parametric and empirical probability distributions to describe the uncertainty about them. This approach allows emissions modelers to assign uncertainty information about an existing inventory without having to change the actual inventory files. The same inventories can be used for both deterministic (i.e., without uncertainty) modeling and stochastic modeling (i.e., with uncertainty), and the type of modeling that is performed depends only on the presence of the additional inventory uncertainty file.

Wang et al. (2000) estimated uncertainties in incremental reactivities for the SAPRC-97 chemical mechanism, with an emphasis on aromatic mechanism parameters, using Monte Carlo analysis with LHS. Rodriguez and Dadbub (2003) performed an MC uncertainty and sensitivity analysis of the Caltech Atmospheric Chemistry Mechanism (CACM), with an emphasis placed on secondary organic aerosol. Uncertainties were propagated through box model simulations.

Hanna et al. (2006) performed a Monte Carlo uncertainty analysis with ISCST3 and AERMOD to study uncertainties in annual average benzene and 1,3-butadiene concentrations in the Houston Ship Channel area caused by uncertainties in meteorological inputs, emissions inputs, and dispersion model parameters.

Martien et al (2006) developed a continuous adjoint sensitivity analysis procedure for a three-dimensional photochemical model to determine the sensitivity of a small number of model responses to many parameters. Menut (2003) also applied an adjoint sensitivity method for a photochemical sensitivity analysis.

Deguillaume et al. (2007) applied a Bayesian Monte Carlo uncertainty analysis to a regional-scale inverse emission modeling study to estimate emission uncertainty in the Ile-de-France region. Deguillaume et al. (2008) applied a Bayesian Monte Carlo analysis to evaluate model uncertainty in ozone production and its sensitivity to emission changes in the CHIMERE model for the Ile-de-France region during the 1998 and 1999 summer seasons. The use of observations to constrain the analysis reduced uncertainty of predicted ozone concentrations.

Response Surface Analysis

Forms of response surface approximations have been used in a variety of scientific, engineering, and economic modeling applications, including groundwater flow using the Stochastic Response Surface Method (SRSM) (Balakrishnan et al., 2003, 2005); radiative forcing by anthropogenic sulfate aerosol Probability Collocation Method (PCM) (Pan et al., 1998); climate change using the PCM (Webster and Sokolov, 2000; Webster et al., 2006), and soil moisture in the NOAA Land Surface Model (Hossain et al., 2004).

Response surface models have been used in the air quality field for the past decade. Calbo et al. (1998) used PCM to develop a parameterization consisting of a set of analytical expressions that approximate the predictions by the CIT Urban Airshed Model. Parameterization development was the ultimate focus of this work, but the authors mentioned that their parameterization was applicable to detailed uncertainty and sensitivity analysis. Isukapalli et al., (1998) applies SRSM to propagate uncertainty through the Reactive Plume Model (RPM-IV). The results agreed closely with those of traditional MC and LHS methods, while significantly reducing the required number of model simulations. Isukapalli et al. (2000) coupled SRSM to the Automatic Differentiation of FORTRAN (ADIFOR) to propagate uncertainty through the Reactive Plume Model (RPM-IV). EPA has developed and used an RSM based on the Community Multiscale Air Quality (CMAQ) model to develop emissions control scenarios in support of the Regulatory Impact Assessment for the PM_{2.5} NAAQS (U.S. Environmental Protection Agency, 2006b).

The response surface method is at the other extreme from simple one-at-a-time sensitivity studies. This method (Tatang et al., 1997) attempts to fit orthogonal polynomials to the input conditions and the predictions of numerical geophysical models. For this approach, it is necessary to run the models a sufficient number of times to have enough data to develop the response surfaces. It is claimed that 25 to 60 times fewer runs are needed than for a MC SRS exercise. However, in a Response Surface Model (RSM) pilot study, Hubbell (2003) reported that 144 REMSAD runs were required to characterize a second order polynomial surface to develop an RSM for PM_{2.5}.

Nevertheless, the response surface is a model of a model and, therefore, is susceptible to problems associated with scenarios outside of the range of parameters used to generate the data for deriving the model.

First-order Sensitivity Analysis

Sensitivity analysis has not been used as extensively as desired because of implementation complexity and computational limitations. As a result, the simple “brute-force” method has been used most frequently to determine model sensitivities, especially in multidimensional chemistry transport models. By this method, a separate simulation is required to calculate the effects of each parameter or emission rate in the model. However, this approach rapidly becomes impractical when a large number of sensitivity coefficients need to be computed.

A number of other approaches have been developed to calculate sensitivity coefficients. One method of reducing this effort is determining the equations governing the sensitivity coefficients and solving them directly. In this method, the sensitivity equations are derived from the model equations and solved simultaneously with the model equations. This method proved to be unstable and inefficient when applied to stiff equations found in many air quality problems (Dunker, 1984). Other techniques rely on Green's function (Rabitz et al., 1983; Cho et al., 1987; Harley et al., 1997) or the adjoint method, in which the sensitivity coefficients are computed from integrals of the Green's function of sensitivity equations derived from the model equations.

The automatic differentiation of Fortran (ADIFOR) technique (Bischof et al., 1992) automatically translates large FORTRAN codes to a subprogram that includes the original functions as well as those for the desired sensitivity coefficients. This method has been used in past studies for sensitivity analysis of the advection equation as used for atmospheric modeling (Hwang et al., 1997), and initial concentrations and reactions rates in photochemical models (Carmichael et al., 1997). Because ADIFOR is designed for general-purpose sensitivity analysis, the expanded codes do not take advantage of the program structure and re-use of calculations. Also, computing some sensitivity coefficients, such as those with respect to the subdomain emissions or the boundary conditions, requires additional modifications that can be cumbersome.

Another approach for computing sensitivity coefficients is the decoupled direct method (DDM) (Dunker, 1981; 1984), in which the sensitivity equations are derived from the model equations, but solved separately. DDM does not share the instability problem found with the direct and adjoint methods. Furthermore, the implementation of this method is more straightforward than the coupled direct or adjoint methods because the sensitivity equations are linear, even though they are functions of concentrations. Therefore, the calculations of sensitivity coefficients are much less computationally demanding. Milford et al. (1992) and Seefeld and Stockwell (1999) also applied the DDM to study variations in chemical rate constants.

Another technique for sensitivity study is DDM-3D (decoupled direct method in three dimensions), which has been successfully implemented in the CIT, CAMx, and CMAQ photochemical AQMs. This approach is highly computation-efficient and capable of calculating a full set of model sensitivity in a three-dimensional domain. Yang et al. (1997) first implemented DDM in a three-dimensional photochemical model (now known as DDM-3D). This implementation was used to calculate first-order ozone sensitivities to dry deposition velocity, initial conditions, rate constants, and NO_x and VOC emissions for a 1987 South Coast ozone episode. DDM-3D was implemented into CAMx version 3.0.0 by Dunker et al. (2002) to calculate first-order ozone sensitivities with respect to emissions and boundary conditions for a 1995 Lake Michigan ozone episode.

Higher-order Sensitivity Analysis

First-order DDM sensitivity analysis is limited because it assumes linear responses to input changes. The use of the higher-order direct decoupled method (HDDM) and its

higher-order coefficients allows DDM to be extended to study non-linear responses, and can be used to study the uncertainty of modeled sensitivities. Most studies that have implemented and tested HDDM have not specifically used the technique to examine uncertainty in pollutant response attributable to uncertainties in inputs.

Hakami et al. (2003) extended DDM-3D to calculate higher-order ozone sensitivities in the MAQSIP photochemical grid model for the 1990 SARMAP domain. HDDM was initially implemented for the CB-IV chemical mechanism, and later extended to the more complex SAPRC chemical mechanism (Hakami et al., 2004). HDDM was ported to CMAQ by Cohan et al. (2005) to CMAQ and applied to a 2001 ozone episode during the Fall Line Air Quality Study. Recently, DDM-3D was extended to calculate first-order sensitivities of PM_{2.5} species in CMAQ (Napelenok et al. 2006).

Hakami et al. (2003) and Cohan et al. (2005) suggested that second-order sensitivity coefficients calculated from HDDM could be applied to quantitatively determine the uncertainty in pollutant sensitivity to uncertain photochemical model inputs. Cohan et al. (2005) used higher-order sensitivity coefficients from HDDM to illustrate how sensitivity and source apportionment estimates can be affected by uncertainty in emissions inventories. Jin et al. (2008) used the second-order sensitivity coefficients from HDDM in CMAQ to assess the influences of uncertainties in various model inputs. Uncertainties in NO_x and anthropogenic VOC emissions, and the rate coefficient for the OH + NO₂ termination reaction were found to have the greatest effect on first-order ozone responses to changes in NO_x emissions.

Though Jin et al. (2008) and Cohan et al. (2005) use HDDM to assess uncertainty, true quantitative uncertainty estimates of pollutant sensitivity to uncertain model inputs remain elusive. An attempt is currently underway to perform a quantitative uncertainty analysis using CMAQ-HDDM, with a Monte Carlo analysis as a post-processor (Digar et al. 2008).

Process Analysis

A technique called process analysis (PA) has been used to assess relative importance of various model assumptions as well as simulated physical and chemical phenomena contributing to an ozone concentration at a particular time and location (Jeffries, 1997; Jeffries et al., 1996; Jang et al., 1995; and Lo and Jeffries, 1997). Because models used to simulate ozone and secondary particulate matter are similar, process analysis should also be useful for addressing PM_{2.5} issues. The technique works by breaking down a modeled simulation into a sequence of physical and chemical processes that lead to a predicted concentration at a given location and time and by tracking the contributions of those processes. PA has been implemented in CMAQ and CAMx but not REMSAD.

While PA requires a substantial amount of expertise to be interpreted to full advantage, useful insights are possible with less detailed analyses. PA takes advantage of numerical grid models that address physical and chemical factors affecting ozone in a sequential manner. For example, a typical sequence followed in a model for each time step might be (1) advection of PM_{2.5} components and precursors present at the beginning of the time

step, (2) PM_{2.5} and precursor emissions added during the time step, (3) vertical diffusion of the advected material and fresh emissions, (4) estimated cloud cover and its effects on photolysis rates, (5) atmospheric chemistry involving advected and diffused material with fresh emissions, and (6) deposition of certain compounds. PA examines incremental effects on changes in component and/or PM_{2.5} predictions from hour to hour attributable to each of the processes described above. In this way, one gets a sense of how important each process is as a contributor to predicted air quality at a specific time and location.

Quantifying Uncertainty in Model Inputs and Options

The first step in uncertainty analysis is to estimate the uncertainties in model input variables and options. Model options may include alternative techniques for solving model equations or alternative physical or chemical submodels. The two primary methods available for the Second Prospective Analysis are literature reviews and expert elicitation. For longer-term efforts in assessing uncertainty, these methods could be supplemented with specific applications of methods already discussed in the literature and in new research.

Literature Reviews

Past and current literature can provide estimates of uncertainties in model inputs based on measurement and sensitivity studies. Because models and measurements are constantly evolving, care must be taken to ensure that estimates of uncertainty in the literature are still valid.

Emission Inventories

Table 1 provides an overview of methods reviewed for the Emission Inventory Improvement Program (EIIP) in its final report on evaluating the uncertainty of emission estimates (Emission Inventory Improvement Program, 1996). While many of the studies cited are now out of date, the report provides a good summary of the methods available for quantifying uncertainty. NARSTO (2005) prepared an assessment of emission inventories across North America. NARSTO's findings on the relative confidence levels for emission inventories are summarized in Table 2.

Additional research has been performed to develop and demonstrate improved methods for quantifying uncertainty in emission inventories. A complete review of research on quantifying uncertainty in emission estimates was not possible within the scope of this work assignment. However, the following discussion provides many examples of the methods used and the results obtained.

In the area of mobile source emissions, Kini and Frey (1997) developed quantitative estimates of uncertainty associated with Mobile5b emission factor model estimates of light-duty gasoline-vehicle base emissions and speed-corrected emissions and found that the uncertainty in average emissions is often $\pm 20\%$ or more. Pollack et al. (1999) performed a similar study on California's EMFAC7G highway vehicle emission factor model. Frey et al. (1999) revisited the earlier analysis of Mobile5b emission factor estimates to include uncertainties associated with temperature corrections. Rhodes and

Frey (1997) quantified variability and uncertainty in AP-42 emission factors using a bootstrap simulation method.

TABLE 1. OVERVIEW OF METHODS FOR EVALUATING THE UNCERTAINTY OF EMISSION ESTIMATES

| METHOD | DESCRIPTION | REFERENCES |
|--|--|---|
| Qualitative Discussion | Sources of uncertainty are listed and discussed. General direction of bias and relative magnitude of imprecision are given if known. | Steiner et al., 1994 |
| Subjective Data Quality Ratings | Subjective rankings based on professional judgment are assigned to each emission factor or parameter. | U.S. EPA, 1995 Saeger, 1994 |
| Data Attribute Rating System (DARS) | Numerical values representing relative uncertainty are assigned through objective methods. | Beck et al., 1994 |
| Expert Estimation Method | Emission distribution parameters (i.e., mean, standard deviation, and distribution type) are estimated by experts. Simple analytical and graphical techniques can then be used to estimate confidence limits from the assumed distributional data. In the Delphi method, expert judgment is used to estimate uncertainty directly. | Linstene and Turoff, 1975 SCAQMD, 1982 Horie, 1988 Horie and Shorpe, 1989 |
| Propagation of Errors Method Direct Simulation Method | Emission parameter means and standard deviations are estimated using expert judgment, measurements, or other methods. Standard statistical techniques of error propagation typically based on Taylor’s series expansions are then used to estimate the composite uncertainty. | Mangat et al., 1984 Benkovitz, 1985 Benkovitz and Oden, 1989 Balentine et al., 1994 Environment Canada, 1994 |
| Direct Simulation Method | Monte Carlo, Latin hypercube, bootstrap (resampling), and other numerical methods are used to estimate directly the central value and confidence intervals of individual emission estimates. In the Monte Carlo method, expert judgment is used to estimate the values of the distribution parameters prior to performance of the Monte Carlo simulation. Other methods require no such assumptions. | Freeman et al., 1986 Iman and Helton, 1988 Oden and Benkovitz, 1990 Efron and Tibshirani, 1991 Environment Canada, 1994 Gatz and Smith, 1995a Gatz and Smith, 1995b |
| Direct or Indirect Measurement (Validation) Method | Direct or indirect field measurements of emissions are used to compute emissions and emission uncertainty directly. Methods include direct measurement such as stack sampling and indirect measurement such as tracer studies. These methods also provide data for validating emission estimates and emission models. | Pierson et al., 1990 Spellicy et al., 1992 Fujita et al., 1992 Peer et al., 1992 Mitchell et al., 1995 Claiborn et al., 1995 |
| Receptor Modeling (Source Apportionment) Method | Receptor modeling is an independent means to estimate the relative contribution of specific source types to observed air quality measurements. The method works best for nonreactive pollutants for which unique emission composition “fingerprints” exist for all significant source categories. The method provides a measure of the relative contribution | Watson et al., 1984 Lowenthal et al., 1992 Chow et al., 1992 Scheff et al., 1995 |

| METHOD | DESCRIPTION | REFERENCES |
|-------------------------------------|--|--|
| | of each source type but not absolute emission estimates. | |
| Inverse Air Quality Modeling Method | Air quality simulation models are used in an inverse, iterative approach to estimate the emissions that would be required to produce the observed concentrations fields. | Hartley and Prinn, 1993 Chang et al., 1993 Chang et al., 1995 Mulholland and Seinfeld, 1995 |

TABLE 2. ESTIMATED RELATIVE CONFIDENCE LEVELS OF EMISSION INVENTORIES.

| SO ₂ | Utilities | high | high | high |
|-----------------|--|-------------|-------------|------------|
| | Other point sources | medium | medium | low-medium |
| | On-road | medium | medium | low |
| | Nonroad mobile | low-medium | medium | low |
| | Stationary nonpoint | low | low | low |
| | Biogenic sources | low | low | low |
| | Other man-made sources (noncombustion) | low | low | low |
| NO _x | Utilities | medium-high | high | medium |
| | Other point sources | medium | medium | medium |
| | On-road | medium-high | medium-high | medium |
| | Nonroad mobile | medium | medium | low |
| | Stationary nonpoint | low | low | low |
| | Biogenic sources | low | low | low |
| | Other man-made sources (noncombustion) | medium | medium | low |
| VOC | Utilities | medium-high | medium-high | medium |
| | Other point sources | low-medium | low-medium | medium |
| | On-road | low-medium | low-medium | low |
| | Nonroad mobile | low-medium | low-medium | low |
| | Stationary nonpoint | low | low | low |
| | Biogenic sources | low | low | low |
| | Other man-made sources (noncombustion) | medium | medium | low |
| HAP | Utilities | medium | medium | medium |
| | Other point sources | low-medium | low-medium | low |
| | On-road | low-medium | low-medium | low |
| | Nonroad mobile | low-medium | low-medium | low |
| | Stationary nonpoint | low | low | low |
| | Biogenic sources | low | low | low |
| | Other man-made sources (noncombustion) | low | low | low |

Bergin and Milford (2000) applied a Bayesian Monte Carlo analysis to estimate uncertainties in ozone concentrations in a Lagrangian photochemical air quality model. Bayesian updating reduced the estimated uncertainty in predicted peak ozone concentrations. Beekmann and Derognat (2003) used a similar approach to analyze uncertainty in a Eulerian photochemical model (CHIMERE). Uncertainties in peak ozone ranged between $\pm 15\%$ and $\pm 30\%$. Measurement constraint reduced uncertainties by a factor of 1.5 to 2.7.

Frey and Bammi (2002) estimated uncertainty in the emission factors for lawn and garden (L&G) equipment. For 2-stroke L&G engines, the 95% confidence intervals for the mean emission factors for total hydrocarbon (THC) and NO_x emissions were -30% to +41% and -45% to +75%, respectively. For 4-stroke L&G engines, the confidence intervals were -33% to +46% for THC and -27% to +35% for NO_x .

Frey and Li (2003) applied quantitative methods for characterizing variability and uncertainty to case studies of emission factors from AP-42 for stationary natural gas-fueled internal combustion engines. The approximate range of uncertainty in mean emission factors varies from as little as $\pm 10\%$ to as much as -60% to +80%, depending on the pollutant, control technology, and nature of the available data.

Frey and Zheng (2002a) developed a probabilistic methodology for quantifying variability and uncertainty in highway vehicle emission factors based on data used in MOBILE5b. Empirical distributions of emissions measurement data were used to characterize variability, while the bootstrap simulation method was used to characterize uncertainty. Inter-vehicle variability in emissions was found to span 2 or 3 orders of magnitude. The uncertainty in fleet average emission factors ranged from $\pm 10\%$ to as much as -90% to +280%.

Frey and Zheng, (2002b) quantified the variability and uncertainty in emission factors and activity factors for power plant NO_x emissions using the Monte Carlo and bootstrap simulation. The uncertainties were then propagated through an emission inventory to produce a probabilistic power plant NO_x emission inventory for North Carolina.

Frey and Bammi (2003) estimated variability and uncertainty in NO_x and total hydrocarbon emission factors for construction, farm, and industrial (non-road) engines. Bootstrap simulations were used to develop confidence intervals for the mean. The 95% confidence intervals for the mean emission factors were as small as -10 to +11% and as large as -48 to +49%, with an average range of -26 to +27%.

Abdel-Aziz and Frey (2003a) used univariate stochastic time series models, and ordinary least-squares regression models were employed to quantify hourly uncertainty in capacity emission factors and heat rate, respectively. The models were used to develop an hourly probabilistic power plant NO_x emission inventory for a four-day period. Abdel-Aziz and Frey (2003b) used multivariate time series models (time series approach) to account for the dependence between emissions from correlated units.

Zhao and Frey (2004) developed probabilistic toxic emission inventories for 1,3-butadiene, mercury, arsenic, benzene, formaldehyde, and lead for Jacksonville,

Florida. Parametric and empirical bootstrap simulations were used to quantify the uncertainty in urban air toxic emission factors. The emission inventory 95% uncertainty ranges were as small as -25% to +42% for chromium to as large as -75% to +224% for arsenic with correlated surrogates. Uncertainty was dominated by only a few source categories. Using a similar approach, Frey and Zhao (2004) developed a probabilistic inventory of urban toxic emissions of benzene, formaldehyde, chromium, and arsenic for Houston, Texas. Maximum likelihood estimation was used to deal with censored (non-detected) values in emission data, and bootstrap simulation in combination with maximum likelihood estimation was used to estimate uncertainty in the mean emission factors. Zhao and Frey (2006) used maximum likelihood estimation and bootstrap simulation to determine asymptotically unbiased mean values and uncertainty for air toxic emission factors. Uncertainty in the mean was also estimated. The largest range of uncertainty in the mean was obtained for the external coal combustion benzene emission factor, with 95th confidence interval of the mean equal to -93% to +411%.

Chi et al. (2004) used bootstrap sampling, expert elicitation, and MC simulations to characterize uncertainty of nonroad emissions for Georgia from the EPA NONROAD model. Tools used were a bootstrap resampling technique and a parametric bootstrap analysis method in Zheng and Frey's Analysis of Uncertainty and Variability Tool (AuvTool). Overall uncertainty ranged from -23 to +33%; however, fuel consumption, growth factors, equipment age distributions, PM and HC speciation profiles, temporal activity adjustments, fuel sulfur effects, and evaporative emissions were not accounted for in the analysis.

Meteorological and Air Quality Models

Derwent and Hov (1988) made estimates of uncertainty in photochemical model inputs based on "best judgments" for an application of sensitivity and analysis techniques. They estimated uncertainties to be $\pm 50\%$ for concentrations aloft; $\pm 30\%$ for emissions and deposition velocities, and hydroxyl radical sinks; $\pm 20\%$ for boundary layer depth; and $\pm 10\%$ wind speed. In preparation for an MC uncertainty analysis of Ozone Transport Assessment Group (OTAG) (1997) modeling, Frey (1998) developed estimates of uncertainty in the AQM inputs based on expert elicitation. Frey reported the uncertainty range, which includes 95% of the data, to be a factor of 5 for initial VOC and NO_x concentrations; a factor of 3 for initial ozone concentrations, boundary conditions of VOC and NO_x, and vertical diffusivity above 1000 m and at times other than 8:00 a.m. to 6:00 p.m.; and a factor of 2 for photolysis rates, cloud liquid water content, rainfall amounts, and emissions except major point sources. The range of uncertainty for chemical reactions in the Carbon Bond IV chemical mechanism varied, by reaction, from a factor of 1.01 to 3.02. The least uncertain model inputs were major point source emissions ($\pm 50\%$), horizontal boundary condition for ozone ($\pm 50\%$), concentrations aloft ($\pm 50\%$), wind direction (± 40 degrees), cloud cover ($\pm 30\%$), vertical diffusivity below 1000 m from 8:00 a.m. to 6:00 p.m. ($\pm 30\%$), relative humidity ($\pm 30\%$), and ambient temperature ($\pm 3^\circ\text{C}$).

Yang et al. (1995) propagated uncertainties in reaction rate parameters, through simulations of urban ozone formation to estimated uncertainties in incremental reactivities of VOCs. Uncertainty ($\pm 1\sigma$) in reactivity ranged from 30% to 70%.

While formal estimates of uncertainty are not typically made of the meteorological model outputs used as inputs to AQMs, some information about uncertainty can be gained from the performance evaluations of these models. Often statistical comparisons of the model predictions to observations are provided. While these statistics provide a first-order estimate of the uncertainty, it must be kept in mind that model estimates and observations may not be spatially and temporally commensurate. Model predictions represent grid-cell volume averages of the predicted parameters at a particular time while observations are most often for a point location and may be averaged over various periods of time. Therefore, model performance-based estimates of uncertainty are likely to be larger than the actual uncertainty.

Olerud et al. (2000) performed meteorological modeling with MM5 for all of 1996 on a grid covering the entire continental United States at 36-km resolution. The results of this modeling have been used by EPA and regional planning organizations (RPOs) in subsequent air quality modeling studies with REMSAD, UAM-V, CAMx, and Community Multiscale Air Quality (CMAQ) model. The root mean square errors for the entire domain were reported by season and ranged from 1.15 to 1.47 m/s for wind speed, 35.2 to 38.5 degrees for wind direction, 2.3°C to 4.2°C for temperature, and 0.8 to 1.7 g/kg for humidity. Doty et al. (2002) reported on meteorological modeling with the RAMS model for the Southern Appalachian Mountains Initiative (SAMI). They found that for their 12-km domain, over all days modeled, the root mean square error for wind speed was 2.18 m/s, the gross error for wind direction was 39 degrees, the gross error for temperature was 1.9°C with a bias of -0.8°C, and the gross error for humidity was 0.8 g/kg with a bias of -0.1 g/kg.

Fish and Burton (1997) performed an uncertainty analysis on a Lagrangian photochemical model applied to stratospheric ozone destruction. Uncertainties in chemical kinetic and photochemical rate data were propagated through the modeling system. Arctic and mid-latitude ozone destruction could be modeled with $\pm 25\%$ and $\pm 50\%$ uncertainty (1 sigma), respectively. It was found that two reactions (out of more than 100) were responsible for more than a third of the uncertainty in the model calculations of Arctic ozone loss.

Moore and Londergan (2001) used a modification of the basic MC method to determine uncertainty. The computationally intensive aspects of the full methodology are replaced by a highly restricted sampling approach that exploits the spatial persistence found in predicted concentration fields. The approach was tested in an application of UAM-IV to assess the uncertainty in the differences in predicted maximum ozone concentration between the base-case and control scenarios. Uncertainty in model inputs and parameters were simulated using stochastic models driven by LHS. They propagated uncertainty in 168 model inputs for emissions, chemistry, meteorology, and boundary conditions.

A probabilistic hourly NO_x emission inventory was developed for 32 units of nine coal-fired power plants in the Charlotte, North Carolina, region for 1995 (Abdel-Aziz and Frey, 2003a,b). The uncertainty was then propagated through the MAQSIP model to estimate the uncertainty in maximum 1-hr and 8-hr concentrations for the Charlotte, North Carolina, modeling domain using an MC simulation (Abdel-Aziz and Frey, 2004). Statistical dependencies between power plant units (inter-unit variability), as well as temporal autocorrelation for each individual unit (intra-unit variability), were accounted for. A total of 50 simulations were performed to represent the ranges of uncertainty in hourly emissions and predicted ozone levels. The range of uncertainty in predicted peak 1-hr ozone concentrations solely attributable to utility NO_x emissions was as large as 25 ppb. Uncertainties in peak ozone concentrations at specific locations could be pinpointed to emissions from a specific power plant. Exceedances of the 8-hr standard were more widespread and not attributable to any one plant.

Mallet and Sportisse (2006) estimated uncertainty in a chemistry transport model due to physical parameterizations and numerical approximations using an ensemble modeling approach. The turbulent closure parameterization and chemical mechanism introduced the highest uncertainties.

Zhang et al. (2007) ran an ensemble of meteorological simulations with perturbed initial conditions through CMAQ to explore the sensitivity of ozone predictions caused by small meteorological perturbations. Significant uncertainties in ozone predictions for the Houston area were attributed to meteorological uncertainties, particularly from wind and temperature.

Expert Elicitation

Quantifying the uncertainties in model input variables may be difficult because there is little specific information on this subject in the literature for the complete spectrum of inputs (e.g., initial and boundary conditions, emissions components, meteorological variables, model parameterization constants, photolysis rates, and chemical rate constants). When quantifying the uncertainties is difficult, Morgan and Henrion (1990) suggest that it is appropriate to carry out an expert elicitation where “experts” are asked to give estimates of uncertainties based on their experience. To combine information from a number of different experts, each expert can be assigned a subjective weight indicating the relative extent of the individual’s expertise with respect to the other experts participating in the elicitation (National Council on Radiation Protection and Measurements [NCRP], 1996). In many instances, each expert may be given equal weight, but in those areas for which the degree of expertise differs markedly, unequal weights may be assigned to each expert.

Hanna et al. (1998) estimated uncertainties in model inputs by taking the median of the uncertainty values (expressed as a plus and minus percentile that would include 95% of the variability) suggested by 10 modelers (experts) who responded to questionnaires. That is, each expert was given equal weight. In that study, no attempt was made to carry

out a comprehensive survey of modelers (experts) or to encourage discussions among modelers.

Hanna et al. (2001) improved on this process by attempting to reach about 100 experts via a web page where the experts could enter their estimates of input uncertainties. The 100 experts included 10 or 20 from each major category of input data (e.g., emissions, boundary and initial conditions, chemical rate constants, and meteorology). However, only about 20 experts responded to the request. It was found that better information could be obtained by meeting with groups of experts at several different laboratories. One reason for the difficulty is that many photochemical modeling experts have not thought much about uncertainties in input parameters and, therefore, the estimates are largely based on intuition and compromise. Hanna et al. suggested that future expert elicitations should be more thorough, including workshops where experts come together to discuss the uncertainties. Experts should also assign weights to themselves based on their degree of expertise. The problem with the approach is that it is time-consuming and resource-intensive (two or three weeks of effort over a time period of about six months plus travel costs for two or three meetings for each of about 20 experts).

Uncertainties in BEIS3 biogenic emission outputs have been thoroughly examined. Hanna et al. (2002) used a Monte Carlo approach, while Hanna and Wilkinson (2004) used an analytical approach. The analytical equations for relative uncertainties agreed approximately with the results of the full Monte Carlo method. The total relative variance in isoprene emissions varied from 0.10 to 0.40, depending on temperature. The total oxygenated volatile organic compounds and monoterpene relative variances were similar, with values ranging from 0.10 to 0.26. They estimated that the relative uncertainty in BEIS3 emissions was in the range of about 0.3 to 0.8 (i.e., $\pm 30\%$ to 80%). Hanna et al. (2003, 2005) evaluated consequences of the BEIS3 uncertainties in chemical transport models (CTMs). The MC uncertainties in the CTM-predicted 1-hr and 8-hr averaged ozone concentrations were studied by drawing 20 random samples from the 1000 sets of BEIS3 outputs and running each CTM (MAQSIP, UAM-V, and URM) 20 times for the three episodes. The estimated total uncertainties of ± 15 to 20% are found to be nearly the same for the three CTMs over the three time periods, for 1-hr and 8-hr averages.

Winiwarter and Rypdal (2001) estimated uncertainty associated with the Austrian Greenhouse Gas emission inventory for CO_2 , CH_4 , and N_2O , and for the overall greenhouse potential. Expert elicitation was used to obtain uncertainties in inventory input data. Error distributions were then developed and combined using MC analysis. Overall uncertainty for all sources and gases was 10.5% and 12% , respectively. Uncertainties were attributed to N_2O emissions from soils, CH_4 from landfills, and CO_2 sinks in forests.

RELIABILITY OF INTEGRATED MODELING SYSTEMS

Much of the available literature on uncertainty in models only addresses the model's sensitivity to model inputs within their range of uncertainty. However, sensitivity to an input does not mean that the sensitivity will influence the IAQMS's response to emission changes. The literature in general indicates that when an IAQMS exhibits reasonable model performance, the system's response to emission changes may be more reliable than its ability to estimate absolute concentrations at monitoring sites.

Relative Response of Models

Hogrefe et al. (2008) suggest that operational model evaluation metrics provide little insight into the reliability of the actual model application in a regulatory setting (i.e., the estimation of relative changes), and that more emphasis should be placed on the development of dynamic evaluation approaches that test model response to changes in emission and meteorology. As a demonstration, Hogrefe et al. (2008) simulated an emission reduction scenario using two different vertical mixing parameterizations. While the model-to-model differences in daily maximum 8-hr ozone concentrations were up to 20 ppb, only minor differences were detected in the relative response of ozone concentrations to emission reductions, resulting in differences of a few ppb or less in estimated future year design values.

Jones et al. (2005) assessed the sensitivity and reliability of the RRF approach in the development of 8-hr ozone attainment plans. They examined the sensitivity of model-predicted responses to emission reductions to the choice of meteorology and chemistry mechanism. The different simulations agreed on whether predicted future-year design values would be above or below the NAAQS threshold at nearly 95% of the monitoring locations in the domain. Jones et al. (2005) also tested the ability of the attainment demonstration procedure to predict changes in monitored ozone design values through a retrospective analysis. An average gross error of around 5 ppb was found between modeled and observed design values. Also, at 27% of sites, model-predicted and observed design values disagreed as to whether the design value was above or below the NAAQS threshold.

Sistla et al. (2004) assert the need to provide uncertainty estimates of predicted RRFs. An operational assessment found that model-to-model differences could introduce an uncertainty in the future estimated design value of 3 to 5 ppb.

Dynamic Evaluation of Models

Dennis et al. (2008) reviews approaches to the evaluation of regional-scale air quality modeling systems, and introduces a conceptual model evaluation framework to provide a context for the evaluation process. The framework involves the complementary application of operational, diagnostic, dynamic, and probabilistic evaluation methods. Methods for each type of evaluation are reviewed, and examples of their application to air quality models are discussed. Data needs for model evaluation are also discussed.

Dennis et al. (2008) suggest that model performance methodologies developed for local and mesoscale model applications during the 1980s and 1990s may not extend for regional-scale applications. Model evaluation criteria should be dependent on the context of the application. Three primary objectives of air quality model evaluation are presented:

1. Determining the suitability of a modeling system for a specific application and configuration.
2. Distinguishing the performance among different models or different versions of the same model.
3. Guiding model improvement.

Dennis et al. (2008) define “dynamic evaluation” as an evaluation that assesses the ability of a model to predict changes in air quality concentrations in response to changes in source emissions or meteorology. A dynamic evaluation requires historical case studies where changes in emissions or meteorology are known, or can be confidently estimated, and the changes in emission or meteorology have a discernable impact on air quality. Cases that potentially meet these criteria include major regulatory programs (e.g., the NO_x SIP Call), cyclical emissions changes (e.g., day-of-the week mobile-source emission changes), and unique events (e.g., the 2003 black out).

Because air quality models are inherently deterministic, they do not explicitly account for uncertainties. A “probabilistic evaluation” attempts to qualify this uncertainty, but no specific widely used prescribed method exists. Ensemble methods are discussed by Dennis et al. (2008), and the authors note that results from a finite set of ensemble simulations are not a true measure of model uncertainty, as they represent only a limited view of a portion of the uncertainty spectrum. Monte Carlo techniques are also briefly discussed, and the authors note that input variables in air quality modeling systems can be correlated, which complicates the interpretation of results. Uncertainty in the model’s relative response to emission reductions is briefly discussed, as are Bayesian approaches, rank order statistics, and extreme value theory. Dennis et al. (2008) conclude that regional air quality modeling systems cannot be validated in the formal sense, but can be shown to have predictive and diagnostic value.

Gilliland et al. (2008) suggest that “dynamic evaluation” is only possible if a retrospective case exists in which substantial emission reductions have resulted in discernable changes in air quality and the change in emissions can be quantified with reasonable confidence. They evaluated the CMAQ model’s ability to predict ozone response to NO_x emission reductions associated with the NO_x SIP Call. Two different post-NO_x SIP Call summer periods were used to address the influence of meteorological changes on the ozone response. Simulations using SAPRC99, CB-IV, and CB-05 were performed to assess the sensitivity of ozone responses to the choice of chemical mechanism. CMAQ underestimated ozone reductions observed after the NO_x SIP Call was implemented. A spatial correlation analysis and comparison with aircraft ozone observations suggested that CMAQ underestimates the contribution of long-range

transport of ozone and its precursors. Simulations using SAPRC more accurately predicted ozone response than simulations using CB-IV.

Recent research on modeling weekend/weekday ozone effects has used models as a tool to assess the causes of these effects for specific urban airsheds; however, they do not really address the issue of using the weekend/weekday as an observational basis for dynamic model evaluations. Yarwood et al. (2003) used CAMx to investigate hypotheses for the causes of weekday/weekend ozone differences in the Los Angeles area. They used first-order sensitivities calculated from DDM-3D in CAMx to study the contributions of VOC and NO_x reductions to weekday/weekend ozone changes. Jimenez et al. (2005) modeled weekend/weekday effects in the northeastern Iberian Peninsula.

Hogrefe et al. (2007) compared CMAQ weekend/weekday changes in ozone to observations. While they noted that weekend/weekday differences existed for observed and modeled ozone during summer 2001, the differences appeared to be mainly attributable to changes in meteorology. The authors suggested that to further compare observed and predicted weekend/weekday differences, methods to remove the effects of meteorological variations on ozone needed to be developed. They outlined steps for future research in this area, as they recognize the potential usefulness of using the weekend/weekday effect as a way to evaluate the modeling system's ability to reproduce observed response to emission changes.

A recent request for proposals from the Coordinating Research Council (CRC Project A-69, "Regional Modeling of Weekday/Weekend Ozone Changes") requires the contractor to perform a dynamic evaluation to test the ability of a regional modeling system to simulate ozone changes in response to weekday/weekend emission changes. They specifically reference Gilliland et al. (2008) as a source of useful approaches.

Marufu et al. (2004) used the August 2003 North American electrical blackout to quantify the direct contribution of power plants to regional haze and ozone. Aircraft observations collected over Pennsylvania, Maryland, and Virginia during the blackout were compared to observations taken during the previous summer in the same locations and under similar meteorological conditions. Marufu et al. (2004) found SO₂ and ozone reductions of 90% and 50% (7 ppb), respectively, and an improvement in visual range of > 40 km.

Hu et al. (2006) used CMAQ DDM-3D model simulations to quantify the effects of power plant emission reductions on SO₂ and ozone during the 2003 blackout. Sensitivity results show that the emission reductions led to SO₂ concentration reductions of 42%, sulfate concentration reductions of 22%, and ozone reductions of less than 5% (2 ppb), and that mobile NO_x emission reductions linked to the blackout had a larger impact on ozone than EGU NO_x emission reductions. The authors use these results to suggest that the observational results from Marufu et al. (2004) are overestimates.

Even though Hu et al. (2006) suggest that the Marufu et al. (2004) observational analysis overestimated ozone response to emission changes induced by the blackout, some recent SIPs (e.g., 2007 Baltimore Ozone SIP, New Jersey Ozone SIP) have used the results of

Hu et al. (2006) as an authoritative argument that CMAQ underestimates ozone response to emission reductions.

UNCERTAINTIES IN THE IAQMS FOR THE SECOND PROSPECTIVE ANALYSIS

The Second Perspective Analysis is the first Section 812 analysis to use an integrated modeling system, the CMAQ model, to simulate national and regional-scale pollutant concentrations and deposition. The CMAQ model (National Exposure Research Laboratory, 1999) is a state-of-the-science, regional air quality modeling system that is designed to simulate the physical and chemical processes that govern the formation, transport, and deposition of gaseous and particulate species in the atmosphere. The CMAQ modeling system was designed to approach air quality as a whole by including state-of-the-science capabilities for modeling multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation. CMAQ was also designed to have multiscale capabilities so that separate models were not needed for urban- and regional-scale air quality modeling.

Douglas et al. (2008) applied the CMAQ model for seven core CAAA scenarios that include four different years that span a 30-year period: 1990, 2000, 2010, and 2020. Scenarios that incorporate the emission reductions associated with the CAA are referred to as with-CAAA while those that do not are referred to as without-CAAA. The scenarios include

- Retrospective Base-year Scenario
 - 1990 without-CAAA
- Base- and Future-year Scenarios without 1990 CAAA Controls
 - 2000 without-CAAA
 - 2010 without-CAAA
 - 2020 without-CAAA
- Base- and Future-year Scenarios with 1990 CAAA Controls
 - 2000 with-CAAA
 - 2010 with-CAAA
 - 2020 with-CAAA

For PM_{2.5} and related species, the CMAQ model was applied in annual simulations for the period January through December. A 36-km resolution modeling domain that encompasses the contiguous 48 states was used for the annual modeling. For ozone and related species, the CMAQ model was applied for a five-month simulation period that captures the key ozone-season months of May through September. Two 12-km resolution modeling domains (that when combined cover the contiguous 48 U.S. states) were used for the ozone-season modeling.

E. H. Pechan & Associates, Inc. (E. H. Pechan & Associates, Inc. and Industrial Economics, Inc. 2006; Wilson et al., 2008) developed the base and projection year

emission estimates that were used in the CMAQ modeling. These emission inventories have several unique features. One is the use of consistent economic assumptions from the Department of Energy's Annual Energy Outlook 2005 (AEO 2005) projections as the basis for estimating 2010 and 2020 emissions for all sectors. Another is the analysis of the different emissions paths for both with and without CAAA scenarios. Other features of this analysis include being the first EPA analysis that uses the 2002 National Emission Inventory files as the basis for making 48-state emission projections, incorporating control factor files from RPOs that had completed emission projections at the time the analysis was performed, and modeling the emission benefits of the expected adoption of measures to meet the 8-hr ozone NAAQS, the Clean Air Visibility Rule, and the PM_{2.5} NAAQS.

Model-ready meteorological input files for 2002 were provided by EPA for use in the CMAQ modeling. The meteorological inputs to CMAQ were developed with the fifth-generation Penn State/NCAR mesoscale model (MM5) (Grell et al., 1994). Dolwick et al. (2007) describe the 36-km and eastern 12-km MM5 modeling and model performance for the eastern 12-km domain. The western 12-km modeling used MM5 meteorology that was developed by the Western Regional Air Partnership (WRAP) (Kemball-Cook et al., 2005). Brewer et al. (2007) described the MM5 model performance on the eastern 12-km domain and a limited analysis of model performance on the 36-km domain. These 2003 meteorological fields were used and described in the technical support document for the final Locomotive/Marine Rule (U.S. Environmental Protection Agency, 2008). The most complete description of the 2002 MM5 evaluation for all domains is in a yet-to-be-released internal EPA document for the entire 2002 CMAQ modeling platform (Dolwick, 2008).

Uncertainties in IAQMS will be assessed using EPA's Response Surface Metamodels (RSMs) for ozone (U.S. Environmental Protection Agency, 2006a) and particulate matter (U.S. Environmental Protection Agency, 2006b). The RSMs are based on an approach known as air quality metamodeling that aggregates numerous pre-specified individual air quality modeling simulations into a multi-dimensional air quality "response surface". Simply, this metamodeling technique is a "model of the model" and has been shown to reproduce the results from an individual modeling simulation with little bias or error over the range of conditions for which they were developed. The RSM incorporates statistical relationships between model inputs and outputs to provide a real-time estimate of air quality changes. The RSM provides a wide breadth of model outputs, which we can use to assess the impact of emission uncertainties. This approach allows for the rapid assessment of air quality impacts of different combinations of emission levels.

While the RSM-based uncertainty assessments have not been documented yet, Table 3 provides an initial description of emissions, meteorological, and air quality uncertainties in the IAQMS based on our review of relevant literature. The literature demonstrates a continuing process of uncertainty identification and reduction over the past several decades. Of the three main components in the IAQMS, the emissions component is still the most complex and uncertain with uncertainties in quantity, composition, spatial and temporal allocation, and future year projection. The literature also shows significant

improvements in the meteorological and air quality modeling components of the IAQMS with more complete and accurate representations of atmospheric physics and chemistry, larger modeling domains, finer grid-resolution, and longer (i.e., annual or seasonal) simulation lengths. The current meteorological models still show regional and season biases in variables that can influence PM_{2.5} formation but the longer term simulations tend to ameliorate the effects of these biases and more clearly define the extent and magnitude of the biases. The air quality model used in the Second Prospective Analysis includes a more complete treatment of aerosol chemistry than used previously but has been shown to underestimate the formation of secondary organic aerosols. The availability of PM_{2.5} measurements (mass and speciation) since the first prospective Analysis has greatly improved our ability to assess model performance and uncertainties in estimates of PM_{2.5}. However, the lack of an available model performance evaluation for the CMAQ 2002 base case modeling limits our ability to understand and quantify the modeling uncertainties and their effects in this analysis.

Uncertainties in Table 3 are separated into broad categories for types of models such as emissions, meteorological, and air quality. In cases where a particular uncertainty is poorly defined or the literature is out of date, the opinions of experts were relied upon to refine the available information. Uncertainties are ranked based on their potential to affect the specific model with which they are associated and their overall effect on the IAQMS response to emission changes.

TABLE 3. UNCERTAINTIES ASSOCIATED WITH THE INTEGRATED AIR QUALITY MODELING SYSTEM IN THE SECOND PROSPECTIVE ANALYSIS.

| CATEGORY ^A | KEY UNCERTAINTIES ASSOCIATED WITH EMISSIONS ESTIMATION POTENTIAL SOURCE OF ERROR | DIRECTION OF POTENTIAL BIAS FOR NET BENEFITS ESTIMATE | LIKELY SIGNIFICANCE RELATIVE TO KEY UNCERTAINTIES IN NET BENEFIT ESTIMATE ^B |
|-----------------------|--|--|---|
| E | Uncertainties in biogenic emissions inputs increase uncertainty in the AQM estimates. Uncertainties in biogenic emissions may be large ($\pm 80\%$). The biogenic inputs affect the emissions-based VOC/NO _x ratio and, therefore, potentially affect the response of the modeling system to emissions changes. | Underestimate. The underestimate of biogenic emissions would reduce overall reactivity leading to underestimates of the model's response to emission reductions. | Potentially major. Impacts for ozone and PM _{2.5} results. Both oxidation potential and secondary organic aerosol formation could influence PM _{2.5} formation significantly. However, ozone benefits contribute only minimally to net benefit projections in this study. |
| E | The With-CAAA scenario includes implementation of the Clean Air Mercury Rule (CAMR), which has been vacated, and Clean Air Interstate Rule (CAIR), which was vacated but has since been remanded. | Overestimate. | Potentially major. Significance in 2020 will depend on the speed and effectiveness of implementing CAIR and replacing CAMR. In some areas, emissions reductions are expected to be overestimated, but in other areas, NO _x inhibition of ozone leads to underestimates of ozone benefits (e.g., some urban centers). |
| E | VOC emissions are dependent on evaporation, and future patterns of temperature are difficult to predict. | Overestimate. | Probably minor. An acceleration of climate change (warming) could increase emissions but the increase over 30 years would not likely be significant. |
| E | Use of average temperatures (i.e., daily minimum and maximum) in estimating motor-vehicle emissions artificially reduces variability in VOC emissions. | Unable to determine based on current information. | Probably minor. Use of averages will overestimate emissions on some days and underestimate on other days. Effect is mitigated in With-CAAA scenarios because of more stringent evaporative controls that are in place by 2000 and 2010. |

| CATEGORY ^A | KEY UNCERTAINTIES ASSOCIATED WITH EMISSIONS ESTIMATION POTENTIAL SOURCE OF ERROR | DIRECTION OF POTENTIAL BIAS FOR NET BENEFITS ESTIMATE | LIKELY SIGNIFICANCE RELATIVE TO KEY UNCERTAINTIES IN NET BENEFIT ESTIMATE ^B |
|-----------------------|---|---|--|
| E | Economic growth factors used to project emissions are an indicator of future economic activity. These growth factors reflect uncertainty in economic forecasting as well as uncertainty in the link to emissions. IPM projections may be reasonable regionally but may introduce significant biases locally. Also, the Annual Energy Outlook 2005 growth factors do not reflect the recent economic downturn or the volatility in fuel prices since the fall of 2005. | Unable to determine based on current information. | Probably minor. The same set of growth factors are used to project emissions under both the Without-CAAA and With-CAAA scenarios, mitigating to some extent the potential for significant errors in estimating differences in emissions. Some specific locations may be more significantly influenced. |
| E | Uncertainties in the stringency, scope, timing, and effectiveness of With-CAAA controls included in projection scenarios. | Unable to determine based on current information. | Probably minor. Future controls could be more or less stringent, wide, or effective than projected. Timing of emissions reductions may also be affected. |
| E | Emissions estimated at the county level (e.g., low-level source and motor vehicle NO _x and VOC emissions) are spatially and temporally allocated based on land use, population, and other surrogate indicators of emissions activity. Uncertainty and error are introduced to the extent that area source emissions are not perfectly spatially or temporally correlated with these indicators. | Unable to determine based on current information. | Probably minor. Potentially major for estimation of ozone, which depends largely on VOC and NO _x emissions; however, ozone benefits contribute only minimally to net benefit projections in this study. |
| E | The location of the emissions reductions achieved from unidentified measures is uncertain. We currently treat these reductions as if they're achieved from non-point sources, but this may not be correct in all cases. | Unable to determine based on current information. | Probably minor. Impacts from these uncertainties would be localized and would not significantly change the overall net benefit estimate. |
| E | The on-road source emissions projections reflect MOBILE6.2 data on the composition of the vehicle fleet. If recent volatility fuel prices persists or if fuel prices rise significantly (like they did in 2007 and 2008), the motor vehicle fleet may include more smaller, lower-emitting automobiles and fewer small trucks (e.g., SUVs). | Underestimate | Probably minor. |

| CATEGORY ^A | KEY UNCERTAINTIES ASSOCIATED WITH EMISSIONS ESTIMATION POTENTIAL SOURCE OF ERROR | DIRECTION OF POTENTIAL BIAS FOR NET BENEFITS ESTIMATE | LIKELY SIGNIFICANCE RELATIVE TO KEY UNCERTAINTIES IN NET BENEFIT ESTIMATE ^B |
|-----------------------|--|---|---|
| M | Unknown meteorological biases in the 12-km western and 36-km MM5 domains due to the lack of model performance evaluations. | Unable to determine based on current information. | Probably minor. Other evaluations using 2002 and similar meteorology and CMAQ have shown reasonable model performance. Although potentially major affects on nitrate results in western areas with wintertime PM _{2.5} problems. |
| M | Known metrological biases in the 12-km eastern MM5 domain. MM5 has a cold bias during the winter and early spring, and has a general tendency to underestimate the monthly observed precipitation. MM5's under prediction was greatest in the fall and least in the spring months. | Unable to determine based on current information. | Probably minor. These biases would likely influence PM _{2.5} formation processes, which was modeled on the 36-km domain. |
| A | Secondary organic aerosol (SOA) chemistry. CMAQ version 4.6 has known biases (underprediction) in SOA formation. | Underestimate. | Probably minor. A significant portion of SOA forms from biogenic emissions. |
| A | The CMAQ modeling relies on a modal approach to modeling PM _{2.5} instead of a sectional approach. The modal approach is effective in modeling sulfate aerosol formation but less effective in modeling nitrate aerosol formation than the sectional approach. | Unable to determine based on current information. | Probably minor in the eastern U.S. where annual PM _{2.5} is dominated by sulfate. Potentially major in some western U.S. areas where PM _{2.5} is dominated by secondary nitrate formation. |
| A | No model performance evaluation of CMAQ for 2002. | Unable to determine based on current information. | Probably minor. Other evaluations using 2002 and similar meteorology and CMAQ have shown reasonable model performance. |

| CATEGORY ^A | KEY UNCERTAINTIES ASSOCIATED WITH EMISSIONS ESTIMATION POTENTIAL SOURCE OF ERROR | DIRECTION OF POTENTIAL BIAS FOR NET BENEFITS ESTIMATE | LIKELY SIGNIFICANCE RELATIVE TO KEY UNCERTAINTIES IN NET BENEFIT ESTIMATE ^B |
|--|--|---|--|
| A | Ozone modeling relies on a 12-km grid, suggesting NO _x inhibition of ambient ozone levels may be under-represented in some urban areas. Grid resolution may affect both model performance and response to emissions changes. | Unable to determine based on current information. | Probably minor. Though potentially major ozone results in those cities with known NO _x inhibition, ozone benefits contribute only minimally to net benefit projections in this study. Grid size affects chemistry, transport, and diffusion processes, which in turn determine the response to changes in emissions, and may also affect the relative benefits of low-elevation versus high-stack controls. |
| A | Emissions estimated at the county level (e.g., low-level source and motor vehicle NO _x and VOC emissions) are spatially and temporally allocated based on land use, population, and other surrogate indicators of emissions activity. Uncertainty and error are introduced to the extent that area source emissions are not perfectly spatially or temporally correlated with these indicators. | Unable to determine based on current information. | Probably minor. Potentially major for estimation of ozone, which depends largely on VOC and NO _x emissions; however, ozone benefits contribute only minimally to net benefit projections in this study. |
| ^a Categories are E (emissions), M (meteorological model), or A (air quality model) ^b The classification of each potential source of error is based on those used in the first prospective Analysis. The classification of “potentially major” is used if a plausible alternative assumption or approach could influence the overall monetary benefit estimate by approximately 5% or more; if an alternative assumption or approach is likely to change the total benefit estimate by less than 5%, the classification of “probably minor” is used. | | | |

The summary tables of key uncertainties that were prepared for the first prospective Analysis (Tables 4 and 5) are provided for comparison to uncertainties in the Second Prospective Analysis. Table 4 includes uncertainties associated with emissions estimation while Table 5 includes uncertainties associated with air quality modeling. Significant improvements are apparent in both the modeling systems and model inputs since the first prospective Analysis was performed. While there have been many improvements in emission inventories the largest improvements have occurred in the air quality modeling system and the availability of PM_{2.5} measurements. The use of longer term simulations with a single “one atmosphere” model in the Second Prospective Analysis significantly reduces many of the original sources of error such as the use of multiple models, different physical and chemical mechanisms, inadequate grid resolution and spatial coverage, and lack of adequate secondary aerosol chemistry. The increased

availability of PM_{2.5} measurements has increased our ability to assess model performance, quantify biases and errors, and gain confidence in the modeling system’s estimates. These improvements have reduced the uncertainty in the IAQMS and the overall analytical chain and allowed us to provide better estimates of the effect and significance of key uncertainties on the net benefit estimate.

TABLE 4. KEY UNCERTAINTIES ASSOCIATED WITH EMISSIONS ESTIMATION IDENTIFIED IN THE FIRST PROSPECTIVE ANALYSIS.

| POTENTIAL SOURCE OF ERROR | DIRECTION OF POTENTIAL BIAS FOR NET BENEFITS ESTIMATE | LIKELY SIGNIFICANCE RELATIVE TO KEY UNCERTAINTIES IN NET BENEFIT ESTIMATE* |
|---|--|--|
| PM _{2.5} emissions are largely based on scaling of PM ₁₀ emissions. | Overall, unable to determine based on current information, but current emission factors are likely to underestimate PM _{2.5} emissions from combustion sources, implying a potential underestimation of benefits. | Potentially major. Source-specific scaling factors reflect the most careful estimation currently possible, using current emissions monitoring data. However, health benefit estimates related to changes in PM _{2.5} constitute a large portion of overall CAAA-related benefits. |
| Primary PM _{2.5} emissions estimates are based on unit emissions that may not accurately reflect composition and mobility of the particles. For example, the ratio of crustal to primary carbonaceous particulate material likely is high. | Underestimate. The effect of overestimating crustal emissions and underestimating carbonaceous emissions when applied in later stages of the analysis, is to reduce the net impact of the CAAA on primary PM _{2.5} emissions by underestimating PM _{2.5} emissions reductions associated with mobile source tailpipe controls. | Potentially major. Mobile source primary carbonaceous particles are a significant contributor to public exposure to PM _{2.5} . Overall, however, compared to secondary PM _{2.5} precursor emissions, changes in primary PM _{2.5} emissions have only a small impact on PM _{2.5} -related benefits. |
| The With-CAAA scenario includes implementation of a region-wide NO _x emissions reduction strategy to control regional transport of ozone that may not reflect the NO _x controls that are actually implemented in a regional ozone transport rule. | Unable to determine based on current information. | Probably minor. Overall, magnitude of estimated emissions reductions is comparable to that in an expected future regional transport rule. In some areas of the 37-state region, emissions reductions are expected to be overestimated, but in other areas, NO _x inhibition of ozone leads to underestimates of ozone benefits (e.g., some eastern urban centers). |
| VOC emissions are dependent on evaporation, and future patterns of temperature are difficult to predict. | Unable to determine based on current information. | Probably minor. We assume future temperature patterns are well characterized by historic patterns, but an acceleration of climate change (warming) could increase emissions. |

| POTENTIAL SOURCE OF ERROR | DIRECTION OF POTENTIAL BIAS FOR NET BENEFITS ESTIMATE | LIKELY SIGNIFICANCE RELATIVE TO KEY UNCERTAINTIES IN NET BENEFIT ESTIMATE* |
|---|---|--|
| Use of average temperatures (i.e., daily minimum and maximum) in estimating motor-vehicle emissions artificially reduces variability in VOC emissions. | Unable to determine based on current information. | Probably minor. Use of averages will overestimate emissions on some days and underestimate on other days. Effect is mitigated in With-CAAA scenarios because of more stringent evaporative controls that are in place by 2000 and 2010. |
| Economic growth factors used to project emissions are an indicator of future economic activity. They reflect uncertainty in economic forecasting as well as uncertainty in the link to emissions. | Unable to determine based on current information. | Probably minor. The same set of growth factors are used to project emissions under both the Without-CAAA and With-CAAA scenarios, mitigating to some extent the potential for significant errors in estimating differences in emissions. |
| Uncertainties in the stringency, scope, timing, and effectiveness of With-CAAA controls included in projection scenarios. | Unable to determine based on current information. | Probably minor. Future controls could be more or less stringent, wide reaching (e.g., NO _x reductions in OTAG region - see above), or effective (e.g., uncertainty in realizing all Reasonable Further Progress requirements) than projected. Timing of emissions reductions may also be affected (e.g., sulfur emissions reductions from utility sources have occurred more rapidly than projected for this analysis). |
| <p>* The classification of each potential source of error reflects the best judgment of the section 812 Project Team. The Project Team assigns a classification of “potentially major” if a plausible alternative assumption or approach could influence the overall monetary benefit estimate by approximately 5% or more; if an alternative assumption or approach is likely to change the total benefit estimate by less than 5%, the Project Team assigns a classification of “probably minor”.</p> | | |

TABLE 5. KEY UNCERTAINTIES ASSOCIATED WITH AIR QUALITY MODELING FROM THE FIRST PROSPECTIVE ANALYSIS.

| POTENTIAL SOURCE OF ERROR | DIRECTION OF POTENTIAL BIAS FOR NET BENEFITS ESTIMATE | LIKELY SIGNIFICANCE RELATIVE TO KEY UNCERTAINTIES IN NET BENEFIT ESTIMATE* |
|--|--|---|
| <p>PM₁₀ and PM_{2.5} concentrations in the East (RADM domain) are based exclusively on changes in the concentrations of sulfate and nitrate particles, omitting the effect of anticipated reductions in organic or primary particulate fractions.</p> | <p>Underestimate.</p> | <p>Potentially major. Nitrates and sulfates constitute major components of PM, especially PM_{2.5}, in most of the RADM domain and changes in nitrates and sulfates may serve as a reasonable approximation of changes in total PM₁₀ and total PM_{2.5}. Of the other components, primary crustal particulate emissions are not expected to change between scenarios; primary organic carbon particulate emissions are expected to change, but an important unknown fraction of the organic PM is from biogenic emissions, and biogenic emissions are not expected to change between scenarios. If the underestimation is major, it is likely the result of not capturing reductions in motor vehicle primary elemental carbon and organic carbon particulate emissions.</p> |
| <p>The number of PM_{2.5} ambient concentration monitors throughout the U.S. is limited. As a result, cross estimation of PM_{2.5} concentrations from PM₁₀ (or TSP) data was necessary to complete the “monitor level” observational data set used in the calculation of air quality profiles.</p> | <p>Unable to determine based on current information.</p> | <p>Potentially major. PM_{2.5} exposure is linked to mortality, and avoided mortality constitutes a large portion of overall CAAA benefits. Cross estimation of PM_{2.5}, however, is based on studies that account for seasonal and geographic variability in size and species composition of particulate matter. Also, results are aggregated to the annual level, improving the accuracy of cross estimation.</p> |
| <p>Use of separate air quality models for individual pollutants and for different geographic regions does not allow for a fully integrated analysis of pollutants and their interactions.</p> | <p>Unable to determine based on current information.</p> | <p>Potentially major. There are uncertainties introduced by different air quality models operating at different scales for different pollutants. Interaction is expected to be most significant for PM estimates. However, important oxidant interactions are represented in all PM models and the models are being used as designed. The greatest likelihood of error in this case is for the summer period in areas with NO_x inhibition of ambient ozone (e.g., Los Angeles).</p> |

| POTENTIAL SOURCE OF ERROR | DIRECTION OF POTENTIAL BIAS FOR NET BENEFITS ESTIMATE | LIKELY SIGNIFICANCE RELATIVE TO KEY UNCERTAINTIES IN NET BENEFIT ESTIMATE* |
|---|---|--|
| <p>Future-year adjustment factors for seasonal or annual monitoring data are based on model results for a limited number of simulation days.</p> | <p>Overall, unable to determine based on current information.</p> | <p>Probably minor. RADM/RPM and REMSAD PM modeling simulation periods represent all four seasons and characterize the full seasonal distribution. Potential overestimation of ozone, due to reliance on summertime episodes characterized by high ozone levels and applied to the May-September ozone season, is mitigated by longer simulation periods, which contain both high and low ozone days. Also, underestimation of UAM-V western and UAM-IV Los Angeles ozone concentrations (see below) may help offset the potential bias associated with this uncertainty.</p> |
| <p>Comparison of modeled and observed concentrations indicates that ozone concentrations in the western states were somewhat underpredicted by the UAM-V model, and ozone concentrations in the Los Angeles area were underestimated by the UAM-IV model.</p> | <p>Unable to determine based on current information.</p> | <p>Probably minor. Because model results are used in a relative sense (i.e., to develop adjustment factors for monitor data) the tendency for UAM-V or UAM to underestimate absolute ozone concentrations would be unlikely to affect overall results. To the extent that the model is not accurately estimating the relative changes in ozone concentrations across regulatory scenarios, the effect could be greater.</p> |
| <p>Ozone modeling in the eastern U.S. relies on a relatively coarse 12-km grid, suggesting NO_x inhibition of ambient ozone levels may be under-represented in some eastern urban areas. Coarse grid may affect both model performance and response to emissions changes.</p> | <p>Unable to determine based on current information.</p> | <p>Probably minor. Though potentially major for eastern ozone results in those cities with known NO_x inhibition, ozone benefits contribute only minimally to net benefit projections in this study. Grid size affects chemistry, transport, and diffusion processes, which in turn determine the response to changes in emissions, and may also affect the relative benefits of low-elevation versus high-stack controls. However, the approach is consistent with current state-of-the-art regional-scale ozone modeling.</p> |

| POTENTIAL SOURCE OF ERROR | DIRECTION OF POTENTIAL BIAS FOR NET BENEFITS ESTIMATE | LIKELY SIGNIFICANCE RELATIVE TO KEY UNCERTAINTIES IN NET BENEFIT ESTIMATE* |
|---|--|--|
| <p>UAM-V modeling of ozone in the western U.S. uses a coarser grid than the eastern UAM-V (OTAG) or UAM-IV models, limiting the resolution of ozone predictions in the west.</p> | <p>Unable to determine based on current information.</p> | <p>Probably minor. Also, probably minor for ozone results. Grid cell-specific adjustment factors for monitors are less precise for the west and may not capture local fluctuations. However, exposure tends to be lower in the predominantly non-urban west, and models with finer grids have been applied to three key population centers with significant ozone concentrations. May result in underestimation of benefits in the large urban areas not specifically modeled (e.g., Denver, Seattle) with finer grid.</p> |
| <p>Emissions estimated at the county level (e.g., area source and motor vehicle NO_x and VOC emissions) are spatially and temporally allocated based on land use, population, and other surrogate indicators of emissions activity. Uncertainty and error are introduced to the extent that area source emissions are not perfectly spatially or temporally correlated with these indicators.</p> | <p>Unable to determine based on current information.</p> | <p>Probably minor. Potentially major for estimation of ozone, which depends largely on VOC and NO_x emissions; however, ozone benefits contribute only minimally to net benefit projections in this study.</p> |
| <p>The REMSAD model underpredicted western PM concentrations during fall and winter simulation periods.</p> | <p>Unable to determine based on current information.</p> | <p>Probably minor. Because model results are used in a relative sense (i.e., to develop adjustment factors for monitor data) REMSAD's underestimation of absolute PM concentrations would be unlikely to significantly affect overall results. To the extent that the model is not accurately estimating the relative changes in PM concentrations across regulatory scenarios, or the individual PM components (e.g., sulfates, primary emissions) do not vary uniformly across seasons, the effect could be greater.</p> |
| <p>Lack of model coverage for acid deposition in western states.</p> | <p>Underestimate.</p> | <p>Probably minor. Because acid deposition tends to be a more significant problem in the eastern U.S. and acid deposition reduction contributes only minimally to net monetized benefits, the monetized benefits of reduced acid deposition in the western states would be unlikely to significantly alter the total estimate of monetized benefits.</p> |

| POTENTIAL SOURCE OF ERROR | DIRECTION OF POTENTIAL BIAS FOR NET BENEFITS ESTIMATE | LIKELY SIGNIFICANCE RELATIVE TO KEY UNCERTAINTIES IN NET BENEFIT ESTIMATE* |
|---|---|---|
| Uncertainties in biogenic emissions inputs increase uncertainty in the AQM estimates. | Unable to determine based on current information. | Probably minor. Potentially major impacts for ozone outputs, but ozone benefits contribute only minimally to net benefit projections in this study. Uncertainties in biogenics may be as large as a factor of 2 to 3. These biogenic inputs affect the emissions-based VOC/NO _x ratio and, therefore, potentially affect the response of the modeling system to emissions changes. |
| <p>* The classification of each potential source of error reflects the best judgment of the section 812 Project Team. The Project Team assigns a classification of “potentially major” if a plausible alternative assumption or approach could influence the overall monetary benefit estimate by approximately 5% or more; if an alternative assumption or approach is likely to change the total benefit estimate by less than 5%, the Project Team assigns a classification of “probably minor”.</p> | | |

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