Arnold Schwarzenegger
Governor

ASSESSMENT OF NITROGEN DEPOSITION: MODELING AND HABITAT ASSESSMENT

PIER FINAL PROJECT REPORT

Prepared For:
California Energy Commission
Public Interest Energy Research Program

Prepared By:
University of California, Riverside

March 2007
CEC-500-2006-032

Prepared By:
University of California, Riverside
Air Pollution Research Center and College of Engineering Center for Environmental Research and Technology

Gail Tonnesen, Zion Wang,
Mohammad Omary, Chao-Jung Chien
Riverside, California
Contract No. 500-99-013
Work Authorization No. 61

Prepared For:
California Energy Commission
Public Interest Energy Research (PIER) Program

Melinda Dorin
Contract Manager

Kelly Birkinshaw
Program Area Manager

Martha Krebs, Ph.D.
Deputy Director
ENERGY RESEARCH AND DEVELOPMENT DIVISION

B. B. Blevins
Executive Director

DISCLAIMER

This report was prepared as the result of work sponsored by the California Energy Commission. It does not necessarily represent the views of the Energy Commission, its employees or the State of California. The Energy Commission, the State of California, its employees, contractors and subcontractors make no warrant, express or implied, and assume no legal liability for the information in this report; nor does any party represent that the uses of this information will not infringe upon privately owned rights. This report has not been approved or disapproved by the California Energy Commission nor has the California Energy Commission passed upon the accuracy or adequacy of the information in this report.

Acknowledgments

The authors acknowledge support from the Western Governors' Association through the Western Regional Air Partnership for developing emissions inventories and other data sets that were adapted for use in this work.

Please cite this report as follows:

Tonnesen, G., Z. Wang, M. Omary, and C. J. Chien. 2007. *Assessment of Nitrogen Deposition: Modeling and Habitat Assessment.* California Energy Commission, PIER Energy-Related Environmental Research. CEC-500-2005-032.

Preface

The Public Interest Energy Research (PIER) Program supports public interest energy research and development that will help improve the quality of life in California by bringing environmentally safe, affordable, and reliable energy services and products to the marketplace.

The PIER Program, managed by the California Energy Commission (Energy Commission), conducts public interest research, development, and demonstration (RD&D) projects to benefit electricity and natural gas customers.

The PIER program strives to conduct the most promising public interest energy research by partnering with RD&D entities, including individuals, businesses, utilities, and public or private research institutions.

PIER funding efforts are focused on the following RD&D program areas:

- Buildings End-Use Energy Efficiency
- Energy-Related Environmental Research
- Energy Systems Integration
- Environmentally Preferred Advanced Generation
- Industrial/Agricultural/Water End-Use Energy Efficiency
- Renewable Energy Technologies
- Transportation

Assessment of Nitrogen Deposition: Modeling and Habitat Assessment is the final project report for the Assessment of Nitrogen Deposition: Modeling and Habitat Assessment project (contract number 500-99-013, work authorization number 61) conducted by the University of California, Riverside. The information from this project contributes to PIER's Energy-Related Environmental Research Program.

For more information about the PIER Program, please visit the Energy Commission's website at www.energy.ca.gov/pier/ or contact the Energy Commission at 916-654-5164.

Table of Contents

Preface ii
Abstract vi
Executive Summary 1
1.0 Introduction 5
1.1. Objectives 5
1.2. Approach 6
1.2.1. Potential Enhancements to Existing Models 7
1.2.2. Ecological Screening 8
2.0 Meteorology and Emissions Inputs 9
2.1. Meteorological Inputs 9
2.2. Emissions Inputs 10
2.2.1. Baseline Emissions Inventory 11
2.2.2. Power Plant Emissions for Sensitivity Case 12
3.0 Description of Air Quality Models Available for use in Deposition Studies 13
3.1. Industrial Source Complex Models 15
3.2. AERMOD 16
3.3. CALPUFF 17
3.4. CMAQ PM/Visibility Modeling Systems 19
4.0 CMAQ and CALPUFF Simulation Results and Discussions 20
4.1. CMAQ Results 21
4.2. CALPUFF Results 29
5.0 Transfer of CMAQ Model Datasets 35
6.0 Conclusions and Recommendations 37
7.0 References 39
8.0 Glossary 41

Appendix A. Description Meteorology Modeling

Appendix B. Development of Emissions Inventory Data for the 4-klm CMAQ Model

Appendix C. Description of Modeling Study Design and Model Configuration

List of Figures

Figure 3-1. Schematic diagram of a Eulerian model. (Figure reproduced from the EPA's CMAQ Users Manual.) (Figure reproduced from the EPA's CMAQ Users Manual.) 14

Figure 3-2. Schematic diagram of a Gaussian dispersion model, illustrating the concentration distribution at two distances (100 m and 300 m) downwind from the emissions source. (Figure reproduced from the EPA's CMAQ Users Manual.) 15

Figure 4-1. 4-km grid resolution modeling domain to be used for the N deposition sensitivity studies in California for both CMAQ and CALPUFF 20

Figure 4-2. Annual total N deposition for the CMAQ air quality model 2002 base case for combined dry deposition and wet deposition 24

Figure 4-3. Annual total N deposition for the CMAQ air quality model 2002 base case for: (top) dry deposition; and (bottom) wet deposition 25

Figure 4-4. CMAQ base case January and July N deposition: dry deposition (top); and wet deposition (bottom). Note different scales in wet deposition plots. 26

Figure 4-5. CMAQ monthly N deposition difference during July between the sensitivity case and base case for dry deposition (top plot) and wet deposition (bottom plot). Note that there is a 10x difference in scale between the two plots. 27

Figure 4-6. CMAQ monthly total N wet deposition difference between sensitivity case and base case for January (top plot) and July (bottom plot) 28

Figure 4-7. CALPUFF model simulated July total N dry deposition for the Metcalf power plant. (Note that the scale in this plot is from -0.001 to 0.001 kg-N/ha/mo) 31

Figure 4-8. CALPUFF model simulated monthly total N dry deposition for January (top) and July (bottom) for the Metcalf power plant 32

Figure 4-9. CALPUFF model simulated monthly total N wet deposition for January (top) and July (bottom) for the Metcalf power plant 33

Figure 4-10. Results from CALPUFF modeling of ambient sulfate concentrations in a separate study performed by ENVIRON Corporation, in which CALPUFF appears to exhibit an artifact of a high concentration spike at significant distances downwind of the source area (figure provided by ENVIRON Corporation). 34

Figure 5-1. Mapping the raster data to the modeling domain 35

Figure 5-2. Dry nitrogen deposition simulated by the CMAQ model in Southern California36

List of Tables

Table 4-1. Summary of total 2002 base case domain-wide emissions; dry, wet, and combined deposition; and ratios for 2002 CMAQ base case 23

Table 4-2. Summary of CMAQ Base Case emissions, dry and wet deposition, and ratios in January and July 23

Table 4-3. Summary of CALPUFF total emissions, dry deposition, and ratios in January and July, 2002 30

Abstract

The Nitrogen Deposition study reviewed four widely used air quality models and concluded that simple Gaussian dispersion models, ISCST3 and AERMOD, are not suitable for modeling N deposition because they fail to represent chemical and phase transformations of nitrogen oxides (NO_X) and ammonia (NH_3) emissions. It reviewed two models that represent chemical speciation and formation of aerosols: CALPUFF and the Community Multiscale Air Quality (CMAQ) model. CALPUFF is a trajectory model that adopts several simplifications that raise important concerns regarding its accuracy. CMAQ is a photochemical grid model and includes state-of-the-art science algorithms. The study performed simulations using each model to assess nitrogen (N) deposition from a power plant. CALPUFF predicted slightly lower deposition rates than did CMAQ, and the spatial features of CALPUFF were poorly resolved. For CMAQ, the study simulated calendar year 2002 to develop baseline N deposition estimates throughout California, and then performed a sensitivity simulation with the new power plant to calculate the change in N deposition. The CMAQ predicted higher deposition rates than the CALPUFF model and provided finer spatial resolution. However, the CMAQ model exhibited numerical noise. The authors recommend exploring other photochemical grid models that might have less numerical noise than CMAQ. Perhaps the most significant outcome of this work is the CMAQ model-simulated baseline annual N deposition for a 4-kilometer resolution grid on a domain that includes much of California. These data have also been converted into an ASCII format that can be readily imported into ArcGIS or other GIS software and used in future ecosystem studies of the effects of N deposition and soil nitrification.

Keywords: CMAQ, CALPUFF, ISCST3, AERMOD, nitrogen deposition, air quality, models

Executive Summary

Introduction

This Nitrogen Deposition research was motivated by previous efforts of the California Energy Commission's biology staff to analyze potential impacts from nitrogen (N) deposition in several power plant licensing cases. Power plants produce emissions of N species, including nitrogen oxides ($NOx=NO+NO_2$) and ammonia (NH_3). These species may deposit to the ground directly or undergo chemical and phase transformation in the atmosphere and be deposited at distances from tens to thousands of kilometers (km) from the source. It is important to quantify the amount and spatial distribution of N distribution because soil nitrification can have harmful effects on N sensitive ecosystems. Several different computer simulation models have been developed for evaluating ambient air quality, and some of these models also represent the deposition of N compounds. However, these air quality models have not been widely applied for assessing N deposition, particularly in arid ecosystems in the western United States, where dry deposition is the dominant form by which N compounds are deposited to soils. Thus, there remains uncertainty in how best to quantify N deposition from new power plants.

Purpose

The purpose of this project was to evaluate several air quality models and to develop recommendations for which models are best suited for simulating the deposition of N from power plants. The evaluation included a review of the science algorithms used in each model and the application of air quality models to compare their predictions of N deposition.

Project Objectives

- Identify air quality models suitable for N deposition modeling.
- Summarize each model's strength, weaknesses, meteorological data requirements, short-distance and long-distance accuracies, and validity of model assumptions.
- Identify potential enhancements to existing models to improve nitrogen deposition impact analysis.
- For those models identified as suitable, perform air quality model simulations to estimate the baseline rates of N deposition in California
- Perform additional model sensitivity simulations to compare modeled estimates of changes in N deposition from new power plant emissions.

Project Outcomes

Section 2 of this report includes a review of four air quality models:

- Industrial Source Complex Short Term (ISCST3) model
- AMS/EPA Regulatory Model (AERMOD)
- CALPUFF, a Lagrangian trajectory model
- Community Multiscale Air Quality (CMAQ), a photochemical grid model.

This study's researchers concluded that that ISCST3 and AEROMOD models were not suitable for modeling N deposition because they fail to represent chemical and phase transformations of NO_X and NH_3 emissions. Because the deposition velocity and uptake by clouds is highly dependent on the chemical form and also the state (i.e., gas or aerosol), the model must represent speciation and aerosol thermodynamics to accurately simulate N deposition. Thus, this study's researchers did not pursue any additional modeling using the ISC and AERMOD models and do not recommend these for use in N deposition studies.

This study also reviewed two models that do represent chemical speciation and formation of aerosols: the CALPUFF model and the Community Multiscale Air Quality (CMAQ) model. CALPUFF is a trajectory model that was developed in the 1980s and adopts several simplifications that raise important concerns regarding its accuracy. The CMAQ model is a recently developed photochemical grid model that includes state-of-the-art science algorithms.

This study's researchers performed simulations in each of these models to evaluate the emissions and deposition of N species from a power plant. CALPUFF predicted slightly lower deposition rates than did CMAQ, and the spatial features of the CALPUFF N deposition were poorly resolved. For the CMAQ model, researchers performed a model simulation for calendar year 2002 to develop baseline N deposition estimates throughout California; and then performed a CMAQ sensitivity simulation with the new power plant and calculated the resulting change in N deposition. CMAQ predicted higher deposition rates than the CALPUFF model and provided much finer spatial resolution. However, the CMAQ model version that was tested also exhibited large numerical noise in the simulated change in N deposition because the increment in N emissions was small relative to the base case N emissions, and because the CMAQ thermodynamics algorithm in this version was prone to developing numerical noise.

Additional products of this work included the development of the input data required to operate the CALPUFF and CMAQ models on a 4-km (2.5 mile, mi) grid for a domain that includes much of California and Nevada. Meteorology input data were developed by performing a simulation of the NCAR/Penn State Mesoscale Model Version 5 (MM5) for calendar year 2002. The MM5 modeling is described in Appendix A. Researchers also developed a comprehensive emissions inventory for the 4-km grid for calendar year 2002. The emissions inventory included all major source categories (e.g., point, mobile, area, biogenic, wildfires) and is described in Appendix B. The emissions inventory data was largely derived from an ongoing air quality modeling study on a 36-km (22-mi) grid that is being funded by the Western Governors' Association. For the N deposition modeling on the 4-km grid, this study developed the new emissions inventories using 4-km resolution spatial surrogate data obtained

from the United States Environmental Protection Agency (EPA). As part of this effort, this study's researchers developed quality control products for the emissions; performance evaluation for the 4-km MM5 and CMAQ simulations, and a comparison of the new CMAQ 4-km model performance to that of the previous WGA 36-km model simulation. These products are available on the project webpage, at http://pah.cert.ucr.edu/aqm/ndep. Perhaps the most significant outcome of this work is the CMAQ model simulated baseline annual N deposition for a 4-km resolution grid on a domain that includes much of California. These data have also been converted into an ASCII format that can be readily imported into ArcGIS or other GIS software and used in future ecosystem studies of the effects of N deposition and soil nitrification.

Conclusions

The authors concluded that the simple Gaussian dispersion models ISCST3 and AERMOD are not suitable for modeling N deposition because they fail to represent chemical and phase transformation of NO_X and NH_3 emissions. The CALPUFF model can be used to simulate N deposition, and its results were generally similar in magnitude to the CMAQ simulated N deposition. However, the CALPUFF produced a more coarsely resolved map of the spatial resolution of N deposition, and there are important concerns regarding the scientific formulation of the CALPUFF model. It was developed in the 1980s and some of its science algorithms are out of date. Furthermore, it uses default or background concentrations of O_3 and NH_3 and this may also affect the accuracy of the CALPUFF simulated N deposition. Thus, uncertainty remains in the CALPUFF modeling results, and further research is needed to test the reliability of these results. Comparisons with future CAMx and CMAQ simulations using the source apportionment algorithms should be useful to investigate these concerns. By contrast, the CMAQ model was developed as a "state-of-the-art" model in the late 1990s and is revised and updated by the EPA each year. However, the CMAQ model versions that were tested (i.e., version 4.3 and 4.4) exhibited numerical noise in sensitivity simulation in which a single point source of emissions is changed. In this study, CMAQ predicted reductions in N deposition in southern California and the authors believe that this is a numerical error in the model.

Recommendations

The ISCST3 and AERMOD should not be used for modeling N deposition. Of the models tested here, the CALPUFF model was the best choice for N deposition modeling because it is numerically stable and requires less resources to operate than the CMAQ model. Although the CALPUFF model did not exhibit problems with numerical noise, it does not fully represent the complexity and nonlinearities in the inorganic system, and there will be large uncertainties in any CALPUFF modeling results. Any model used for studying N deposition must be capable of treating the full complexities of the inorganic system. Therefore, this study's authors recommend that other photochemical grid models should continue to be evaluated for N deposition modeling. The EPA released an updated version of the CMAQ model (version 4.6) in fall, 2006. The update is expected to correct problems with numerical instability in the CMAQ ISORROPIA thermodynamics solver, and this might correct the problems with numerical noise that were observed using the older version of CMAQ. ENVIRON Corporations CAMx model is another widely used air quality modeling, it has low numerical noise, and it also simulates wet

and dry deposition of N species. Both the current version of CAMx and CMAQ 4.6 should be evaluated in future studies.

An important conclusion that stems from this work is that further testing is needed if California is serious about studying incremental nitrogen deposition for ecological effects. None of the models tested in this study were deemed adequate.

Benefits to California

This work benefits California by providing recommendations for air quality models that can be used to assess N deposition resulting from power plants N emissions. This work also provides a model simulated estimate of N deposition throughout most of California with a spatial resolution of 4-km. These data have been shared with other researchers who are investigating ecosystem effects of N deposition. These results and data sets will be valuable in studying the effects of N deposition on sensitive ecosystems in California and in developing guidance to mitigate the effects of N deposition from new power plants, and to preserve California's unique plants and ecosystems.

1.0 Introduction

This research was motivated by previous efforts of biology staff at the California Energy Commission (Energy Commission) to analyze potential impacts from nitrogen (N) deposition in several power plant licensing cases. These power plants were located in areas with N-poor soils and N-sensitive plant communities. Such communities are often rare and support many of California's rare and endangered plant and animal species. Nitrogen saturation has several detrimental effects on these plant communities, including decreased plant function due to leached nutrients (e.g., calcium) from the soil; loss of fine root biomass; decreases in symbiotic mycorrhizal fungi; promotion of exotic invasive species; and leaching into surface waters and ground waters, which increases acidification. Because of the negative effects of soil nitrification it was desirable to estimate the changes in N deposition that would occur as a result of these new power plants. It was also expected that future siting cases may need to review the impact of power plant emissions on nitrogen-saturated or nitrogen-limited ecosystems. Generally, the Energy Commission is interested in assessing impacts to terrestrial ecosystems from nitrogen deposition during power plant commissioning and operation and understanding the validity, strengths, and weaknesses of models used to determine this impact. Specifically, the Energy Commission seeks to better characterize the short-distance and long-distance nitrogen deposition impacts to nitrogen-limited habitats and the species dependent upon those habitats.

The common theme in each of the Energy Commissions' power plant licensing cases was a debate over the more appropriate model for use in assessing nitrogen deposition impacts; either the Industrial Source Complex Short Term (ISCST3) model or the CALPUFF air quality dispersion model. Both of these models describe the relationships between N emissions rates and certain factors affecting the dispersion and dilution in the atmosphere and deposition of N compounds. Both models can also provide estimates of the area most influenced by emissions from a particular source. However, there are major differences in the approach and in the physical processes represented by these models. Moreover, ISCST3 and CALPUFF are only two of many air quality models available, and it is likely that debate over which model to use to assess N and other deposition impacts will continue as more models and model updates become available. Thus, biology staff, power plant applicants, and other stakeholders required a critical review of the strengths, weaknesses, and assumptions of each model; and also recommendations of which air quality models should be used to determine nitrogen deposition in future power plant licensing cases.

1.1. Objectives

The goal of this research was to provide a critical review of the major air quality models that have been proposed for use in evaluating power plant emissions of nitrogen oxides (NO_x=NO+NO_2) and ammonia (NH_3), including their release rate, ambient concentrations, dispersion, chemical transformations, and deposition rates at ground level. Specific objectives included the following:

- Identify air quality models suitable for N deposition modeling
- Summarize each model's strength, weaknesses, meteorological data requirements, short-distance and long-distance accuracies, and validity of model assumptions
- Identify potential enhancements that might be made to future versions of existing models to improve nitrogen deposition impact analysis

- For those models identified as suitable, perform air quality model simulations to estimate the baseline rates of N deposition in California
- Perform additional model sensitivity simulations to compare modeled estimates of changes in N deposition from new power plant emissions

In a related project under separate Energy Commission funding, researchers at the University of California (UC) Santa Barbara provided: (1) an assessment of nitrogen-limited habitats that could be at higher risk from further nitrogen deposition, and (2) location of nitrogen saturated soils/ecosystems in California.[1]

1.2. Approach

The study began with a critical review of the science algorithms used to treat N partitioning and deposition in each of four available models:

- The Industrial Source Complex Short Term (ISCST3) and AERMOD Gaussian Dispersion models
- The CALPUFF photochemical trajectory model
- The EPA's Community Multiscale Air Quality (CMAQ), a photochemical grid model

It is well known that the deposition velocity and transport range of N varies considerably, depending on the chemical form of the N species. Emissions of NO_x are primarily in the form of nitric oxide (NO) which has a relatively slow deposition velocity and long transport range. Emissions of NO can be rapidly oxidized to nitrogen dioxide (NO_2), and subsequently to gas phase nitric acid (HNO_3), peroxyacetyl nitrates (PAN), and organic nitrates (RNO_3). Gas-phase HNO_3 also reacts with ammonia (NH_3) to form aerosol ammonium nitrate. Because HNO_3 and NH_3 have very rapid deposition velocities and short transport ranges, while aerosols and other N species have intermediate or slow deposition velocities, it is essential to accurately characterize the partitioning of N emissions among the several gas phase and aerosol forms. Moreover, meteorology determines the rate of N transport and also profoundly affects the rate of chemical transformation. Finally, the rate of NO oxidation has a complex dependence on the emissions of NO_x, volatile organic compounds (VOCs), and other species that effect the chemical transformations. Thus, physically realistic chemical transport models must be used to represent the transformations and fate of N species.

A variety of chemical transport models are available, and any of these could be used to simulate the deposition of N species. At the simplest level, upper and lower bounds for N transport distance can be determined using the ISCT3 model by assuming that all NO_x is in the form of either NO or HNO_3 and that all ammonia is in either the gas phase or aerosol form. A more accurate determination requires the use of a chemical transport model that simulates the partitioning of N among gas phase and aerosol species. The CALPUFF model uses highly simplified chemistry to attempt to represent N partitioning with relatively low computational cost. More complex and realistic models include the Regulatory Modeling System for Aerosols and Deposition (REMSAD) and the U.S. Environmental Protection Agency's (EPA's) Models-3

---

[1] Weiss, S. B. 2006. *Impacts of Nitrogen Deposition on California Ecosystems and Biodiversity.* California Energy Commission, PIER Energy-Related Environmental Research. CEC-500-2005-165.
.

Community Multiscale Air Quality modeling system (CMAQ). Although direct comparisons of these models have not yet been performed for N deposition, it is likely that they would produce substantially different predictions in the partitioning and transport range of N.

This project performed model comparisons between CALPUFF and CMAQ for several different meteorological scenarios. Model simulations were compared to monitoring data for N species and deposition. After completing the initial model comparison, the researchers selected one model to operate for an annual simulation, which provided estimates of N deposition for a variety of meteorological and seasonal conditions.

Meteorological data were produced by operating the National Center for Atmospheric Research (NCAR)/Penn State Mesoscale Model (MM5) for the year 2002 on a 4-km (2.5 mile) resolution grid for Central California. The modeling domain is illustrated in Figure 4-1. Emissions inventories were derived from previous ozone (O_3) and particulate matter (PM) modeling studies for Central California (Tonnesen et al. 2003a) and for the western United States (Tonnesen et al. 2002).

Prior to this work, this study's researchers were already performing annual modeling of fine particulates using MM5 and CMAQ under funding from the Western Governors' Association for a 36-km (22 mile) grid for the continental United States. The high-resolution 4-km meteorology and emissions data was nested in the 36-km data sets. Emissions data for the 4-km nested grid was prepared from emissions data used in the 36-km modeling. The Sparse Matrix Operator Kernel (SMOKE) emissions processing system was used to prepare the 4-km emissions, and these datasets were compared with 4-km Central California Ozone Study (CCOS) 2000 emissions data as a quality assurance (QA) measure.

Researchers performed two sets of simulations: (1) a baseline estimate of N deposition using current 2002 NO_x and NH_3 emissions, and (2) a sensitivity case to evaluate the effects of adding new N emissions sources at selected locations. This study's researchers used this approach previously in model simulations of the effects of backup diesel generators on air quality in California (Tonnesen et al. 2003b). Results of model deposition estimates were converted to annual N deposition totals in ArcInfo format to facilitate subsequent analysis with plant species population data, similar to that shown in Fenn et al. (2003, Figure 5).

The modeling phase produced three beneficial results:

1. A critical review of science algorithms in the CALPUFF and CMAQ models
2. A comparison of N deposition estimates in CALPUFF and CMAQ for several meteorology scenarios
3. A cumulative annual N deposition estimate in ARCINFO format for a baseline N emissions scenario and for a sensitivity case with additional N sources added at selected locations.

1.2.1. Potential Enhancements to Existing Models

The land use data in the CMAQ model is assigned for each 4-km grid cell according to the dominant land use type within the 4-km grid cell. This study explored the possibility of using sub-grid resolved land use and vegetation type data to refine the deposition velocity estimates to 1-km (0.6-mi) resolution. This approach is conceptually simple and can be described as a "mosaic" approach. It would require specifying high resolution land use data, recalculating the

surface roughness and deposition velocities for each sub-grid land use type, and calculating an averaged deposition velocity proportionally weighted by the fractional area of each land use type within the grid cell. Then, a post processing program could be used to reattribute the N deposition in each grid cell to the sub-grid resolved land use types. In practice, there are several obstacles to implementing this approach. It would require each of the following tasks:

- Obtaining 1-km land use and vegetation data.
- Redoing the MM5 simulation using sub-grid resolved land use data.
- Redoing the pre-processing of the MM5 data using the CMAQ Meteorology Chemistry Interface Package (MCIP). This would require extensive modifications to MCIP to calculate sub-grid resolved surface roughness and deposition velocities as a function of land-use, and to create a composite deposition velocity.
- Developing a post processor to reassign the mean deposition for each grid cell to the sub-grid resolved land-use data.

All of the above tasks are feasible, but it would require a major effort to implement and test this approach, and it is beyond the scope of the current project. However, the EPA is considering the feasibility of implementing some of these approaches in future versions of the CMAQ model.

1.2.2. Ecological Screening

Results from the N deposition modeling study were used in a separate study by Dr. Stuart Weiss (Bren School of Environmental Management, UC Santa Barbara,) for ecological screening of habitats and species. Specific goals of that study included the following:

- Provide a review of existing information and research on the effects of nitrogen deposition on sensitive habitats in California.
- Provide an assessment of nitrogen-limited habitats and nitrogen-saturated soils/ecosystems in California and identify the associated sensitive species.
- Identify, map, and briefly describe life history requirements of species, identifying special status species dependent upon these habitats.

2.0 Meteorology and Emissions Inputs

2.1. Meteorological Inputs

Meteorology data is a key input data that is required for running any air quality model. These data include wind speed and direction, atmospheric stability and vertical motion in the atmosphere, sunlight intensity, clouds and precipitation, and information about mixing at the ground surface, which is required for estimating removal of atmospheric pollutants by dry deposition. Meteorology data can either be developed from observational data or by operating numerical simulation models. For use in Gaussian dispersion models, the modeler simply provides as input data the Briggs atmospheric stability class at a single point, based on observed wind speed and sunlight intensity. More sophisticated approaches employ numerical simulation models to develop explicit, time-resolved meteorology data over a grid of regularly spaced nodes that encompass the models spatial domain.

There are two basic types of numerical meteorology models: diagnostic and prognostic. Diagnostic models interpolate between observed data points to develop gridded and time-resolved data. An example of a diagnostic meteorology model is the CALPUFF model (Scire et al. 2000). The advantage of diagnostic models is that they are relatively simple to operate. Disadvantages are that their accuracy is severely limited by the amount and quality of available observations. Prognostic models address these problems by solving the fundamental equations governing conservation of mass, energy, and momentum. An example of a prognostic model is the Mesoscale Model Version 5 (MM5) (Grell et al. 1994). Although prognostic meteorology models such as MM5 can also exhibit large errors and bias, prognostic models are more accurate than diagnostic models and are recommended for use in gridded air quality modeling studies. The primary disadvantage of using the MM5 model is its greater complexity and operating cost.

Both the CALPUFF and CMAQ air quality models, described in Section 3, require meteorology data as inputs. Gridded meteorological data is required as input data for the CMAQ model, while the CALPUFF model has the option to used observational meteorological data or gridded meteorological data if it is available.

New 2002 annual 4-km meteorological data needed to be developed in this project for the CMAQ and CALPUFF model simulations. Appendix A describes the sources of meteorology data and how it was processed through the PSU/NCAR Mesoscale Model version 5 (MM5) to produce the required 4-km meteorological fields. To summarize, the researchers had previously completed calendar year simulations of the MM5 on a 36-km grid for the continental United States (Kembell-Cook S., et al. 2005). In this study, the researchers performed an additional MM5 simulation on a high resolution, 4-km grid for a modeling domain that included most of California. The operation of the MM5 for the 4-km domain is described in more detail in Appendix A.

Any data set generated by a meteorological model for use as input to an air quality model should first be compared with observational meteorological data, including surface and upper air observations. For the MM5 evaluation the researcher extracted hourly observation data from the University Corporation for Atmospheric Research (UCAR) Techniques Development Laboratory (TDL) datasets, and these were used to compare with the MM5 model results. A summary of the 4-km MM5 evaluation is included in Appendix A. Comparisons between the WRAP 36-km MM5 evaluation and the new 4-km MM5 evaluation for the California domain show that the 4-km domain produced a slightly larger bias for wind speed, wind direction, and

temperature. It is likely that the poorer performance of the 4-km MM5 was a result of using fewer layers in the 4-km MM5 (19 layers) compared to the 36-km MM5 (34 layers), and because observation nudging was not used in the 4-km simulation. However, the research team concluded that the differences are not large enough to cause major concerns with the 4-km MM5 simulation results

After the meteorological fields were produced with MM5, the Meteorological Chemical Interface Processor (MCIP) was used to generate meteorological fields for CMAQ, and the CALMM5/CALMET preprocessors were used for CALPUFF. The post-processing of the MM5 outputs with MCIP and CALMET is described in Section 4.

2.2. Emissions Inputs

Emissions inventory data is a key input to the air quality model, and the model simulated N deposition is probably more sensitive to uncertainty in the emissions than any other input because the total N deposition is directly related to the influx of N compounds from the emissions.

For this project, it is useful to think of two different aspects of the emissions inventory. First, there are emissions of NO_x, NH_3 and other species from a particular power plant which maybe under review for permitting at a particular site. These emissions would represent some increment to the total or "baseline" emissions inventory and some increment to the baseline N deposition rate. Second, there is the baseline emissions inventory, which is comprised of many different types of emissions sources over a large region. In some regions of California with large agricultural emissions of NO_x and NH_3, the baseline N deposition rate can be larger than 10 kilograms of N per hectare per year (kg-N/ha/year) (Fenn et al. 2005) Depending on the location of the new power plant, it can represent either a small increase or a large increase in N deposition rates over the baseline values.

The baseline emissions inventory also creates an ambient chemical environment that effects the chemical transformations and deposition rate of emissions from a power plant. For example, power plant emissions of NO_x in a pristine environment would be slowly oxidized to HNO_3 and would be transported over longer distances and a larger area before being deposited. In an urban influenced environment, however, NO_x would be rapidly converted to HNO_3 and would tend to be deposited closer to the power plant. An inverse relationship may exist for power plant emissions of NH_3. In a pristine environment a larger fraction of NH_3 is likely to remain in the gas form and deposit rapidly, while in an urban influenced environment NH_3 will react with sulfuric and nitric acid to form ammonium aerosol and will deposit more slowly and at greater distances. (However, even in a pristine environment, some NH_3 will interact with sulfate from a power plant plume to form ammonium sulfates.) Thus, to model the fate of emissions from a particular power plant accurately, it is necessary to have a complete baseline emissions inventory and to simulate correctly the ambient chemical environment into which the power plant emissions are injected.

Development of a complete baseline emissions inventory is a difficult and resource intensive task because of the many types and large number of emissions sources that form the inventory. A variety of databases and emissions models must be used to generate the inventory. Additional processing of the inventory is also required to convert it to a gridded, speciated, and temporalized format that can be used by an air quality model. For example, an emissions model might produce an emissions estimate of tons of VOC per county per year. These emissions must

then be processed to provide individual organic species with hourly resolution in the spatial gridding system and binary data format being used by the air quality model.

This study uses emissions inventory data that the research team previously developed as part of a study funded by the Western Governors' Association to simulate annual air quality and visibility for calendar year 2002. This modeling was done on 36-km and 12-km grids over a spatial domain that included the continental United States, and the 13 western states, respectively. This effort is still in progress and is being performed through the WGA's Western Regional Air Partnership (WRAP). The advantage of using the WRAP emission databases is that WRAP and other Regional Planning Organizations (RPOs) have devoted substantial resource to developing improved emissions inventories specifically for the calendar year 2002 visibility modeling. Because errors and uncertainty in emissions inventories are the most important sources of uncertainty in air quality modeling studies, this N deposition study benefited from these efforts by using the RPO grid.

2.2.1. Baseline Emissions Inventory

Emissions input data for the Energy Commission 4-km domain were based on emissions data developed for the WRAP 2002 36-km emissions datasets. The emissions for the following source categories were processed for the calendar year 2002:

1. Area source emissions
2. Point source emissions
3. Mobile emissions
4. Non road mobile emissions
5. Road dust
6. Off shore sources
7. Mexico emissions inventory
8. Biogenic emissions for VOC

Point source emissions include geographical locations in latitude and longitude, and these data were reprocessed for use in the 4-km grid. For biogenic emissions, researchers operated the EPA's Biogenic Emissions Inventory System (BEIS3), using 36-km land use and meteorology data to develop the annual biogenic inventory. The 4-km land use resolution data was not available so researchers downscaled from the 36-km emissions inventory by distributing the emissions from each 36-km grid cell equally among the eighty-one 4-km grid cells located within each 36-km cell. For all other sources, researchers used spatial surrogate gridding data developed by the EPA based on population data to locate county-based emissions data into the appropriate 4-km grid cell.

For all of the emissions processing, this study used the EPA's Sparse matrix Operator kernel emissions (SMOKE) processing system. Additional descriptions of the emissions processing systems and the procedures used to develop the 2002 4-km emissions inventory are included in Appendix B. Processing emissions inventory data is a difficult, tedious, and error-prone task. Therefore, quality assurance (QA) of the processed emissions data is a critical step in performing air quality modeling studies. This study developed extensive QA plots

summarizing the processed 4-km annual emissions in a variety of formats. These include the following:

- Daily total emissions spatial plots for each species
- Domain total diurnal time-series plots for each species
- Annual time-series plots showing domain total daily emissions for each species
- For elevated point and fire sources, daily vertical layer emissions profiles

Appendix B summarizes the QA products, which are also presented in detail on the project webpage at: http://pah.cert.ucr.edu/aqm/ndep/qa_cec2002.shtml.

2.2.2. Power Plant Emissions for Sensitivity Case

For the model sensitivity cases designed to evaluate the effects of a particular power plant, researchers developed a new annual emissions inventory that included emissions from a hypothetical new power plant. The power plant emissions were developed based on data provided by Energy Commission staff for a source named "Metcalf Energy Center." The annual total emissions for this source were 28 tons/yr VOC; 123.4 tons/yr NO_x; 588 tons/yr CO; 10.6 tons/yr SO_2; and 91.3 tons/yr $PM_{2.5}$. The source location was latitude 37.2815 and longitude -121.9598. This was located in column 26 and row 165 of the modeling domain shown in Figure 4-1. This source did not include NH_3 emissions. The NO_x emissions mass are calculated on an NO_2 basis. When converted to an N basis, the NO_x emissions were 37.6 tons-N/yr, or 34,142 kilograms of nitrogen per year (kg-N/yr). For comparison, the domain total, annual, baseline N emissions from all sources is 7.3×10^{11} kg-N/yr. Thus, the additional source added in the model sensitivity simulations was small compared to total N emissions.

3.0 Description of Air Quality Models Available for use in Deposition Studies

Air quality models are designed to represent the chemistry and transport of traces gasses and particulate matter for each trace chemical species (C_i) present in the atmosphere. Typically, air quality models employ the mass continuity equation to write a partial differential equation, including the following terms, for each species i:

- Emissions of trace chemical species (E_i)
- Advective transport by mean wind velocity ($\nabla \cdot \mathbf{V} C_i$)
- Dispersive transport caused by atmospheric turbulence ($\nabla \cdot \mathbf{D} \nabla C_i$)
- Photochemical transformations in gas phase chemistry and heterogeneous chemistry in aqueous or particulate aerosols, which can be represented as chemical production $P_i(\mathbf{C})$ and chemical loss ($L_i(\mathbf{C})C_i$)
- Removal of pollutants by wet and dry deposition (D_i)

Conservation of mass allows an equation to be written for each species i:

$$\frac{\partial C_i}{\partial t} + \nabla \cdot \mathbf{V} C_i = -\nabla \cdot \mathbf{D} \nabla C_i + P_i(\mathbf{C}) - L_i(\mathbf{C}) C_i + E_i + D_i \qquad \text{for } i = 1, N \qquad (1)$$

where N is the number of species represented in the air quality model, and ∇ represents the gradient or 3-dimesional spatial derivative. Equation 1 produces a system of N non-linear, partial differential equations (PDE) that are coupled by the chemical species concentration vector ($\mathbf{C}$). Air quality models that employ Equation 1 are known as *Eulerian models* after the eighteenth century mathematician Leonhard Euler who first developed methods for solving Equation 1. Figure 3-1 illustrates the 3-dimesional frame of reference for Eulerian models in which mass transfer is calculated between adjacent grid cells. Because Eulerian models are defined on a 3-dimesional grid mesh, they are commonly referred to as *grid models.* Typical applications of grid models employ a grid mesh with on the order of 100 by 100 grid cells in the horizontal dimension and between 10 to 30 layers in the vertical dimension.

Although Equation 1 cannot be solved analytically, numerical methods can be used to obtain highly accurate, approximate solutions. However, Equation 1 is computationally expensive to solve. Indeed, until recently it was not possible to solve Equation 1 for the long-term scenarios required for modeling the transport and fate of trace species for evaluating ecosystem effects.

Two different approaches have been used to simplify Equation 1 and to reduce the computational cost of air quality models. In *Lagrangian models,* the frame of reference is defined by the wind vector, and dispersion or mass transfer between air parcels is neglected. This assumption reduces Equation 1 to a system of ordinary differential equations (ODEs) that are solved for each parcel of air:

$$\frac{dC_i}{dt} = \mathbf{D} \frac{d^2 C_i}{dt^2} + P_i(\mathbf{C}) - L(\mathbf{C}) C_i + S_i \qquad \text{for } i = 1, N \qquad (2)$$

This greatly simplifies the numerical solution of the model because the model can be solved for a single air parcel, or for a relatively small set of air parcels compared to the large number of grid cells used in Eulerian models. However, Lagrangian models can still be computationally expensive because of the high cost of achieving accurate solutions of the photochemistry and aerosol thermodynamics in Equation 2. Additional simplifications have been used in some Lagrangian models, such as CALPUFF, to further reduce computation cost by employing lookup tables or default concentration fields for some chemical species.

An additional simplification can be achieved for non-reactive pollutants for which chemical reaction can be neglected. Gaussian dispersion models neglect chemistry and employ a parameterized characteristic plume dispersion profile that is based on measurements of typical plume dispersion in field studies. Figure 3-2 illustrates the conceptual design of Gaussian dispersion models, in which the dispersion of the plume from a point source is assumed to vary as a function of the downwind distance from the point source. Examples of Gaussian dispersion models include the Industrial Source Complex model (ISC) and the AERMOD model. These models can only be used for non-reactive pollutants, or for pollutants that have simple chemistry with linear rates of decay. The model simulated N deposition for the baseline and sensitivity case is discussed in Section 4.

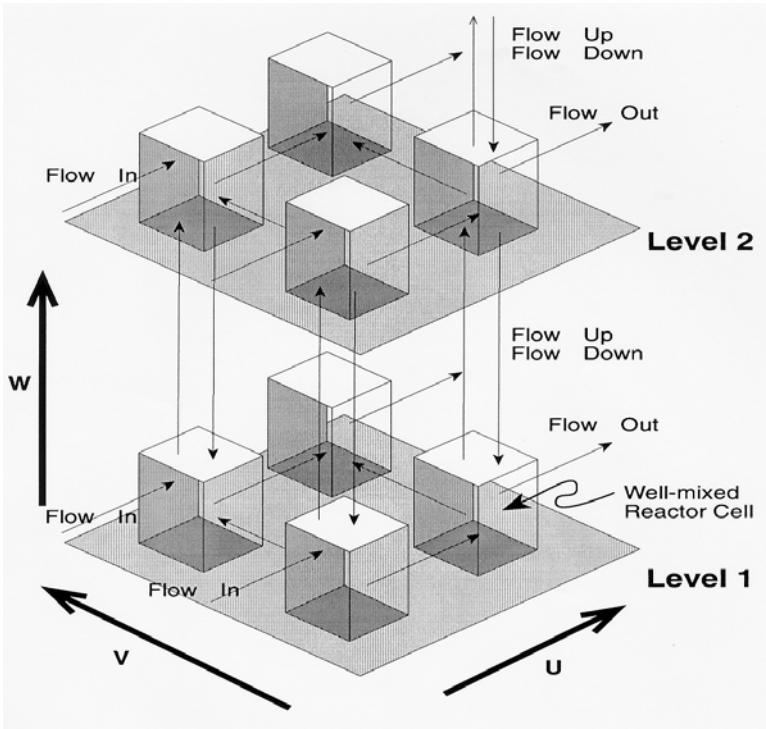


Figure 3-1. Schematic diagram of a Eulerian model. (Figure reproduced from the EPA's CMAQ Users Manual.) (Figure reproduced from the EPA's CMAQ Users Manual.)

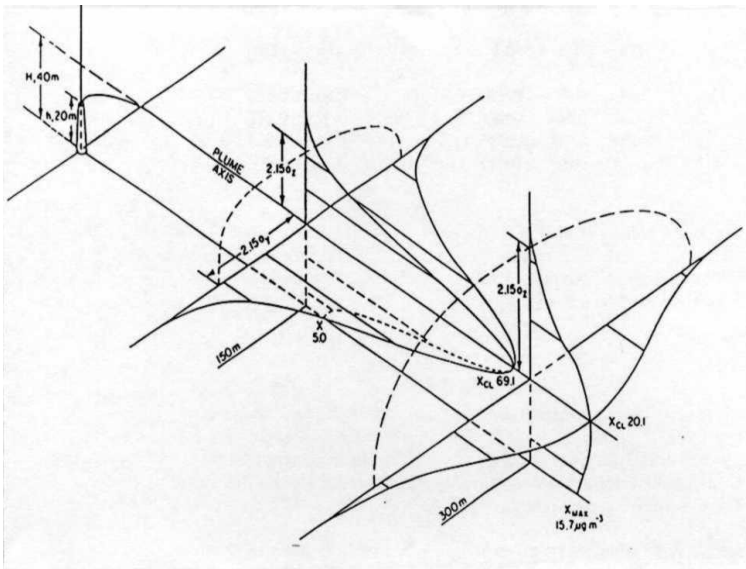


Figure 3-2. Schematic diagram of a Gaussian dispersion model, illustrating the concentration distribution at two distances (100 m and 300 m) downwind from the emissions source. (Figure reproduced from the EPA's CMAQ Users Manual.)

3.1. Industrial Source Complex Models

The Industrial Source Complex model (ISC) is a Gaussian dispersion model recommended in the EPA's *Guideline on Air Quality Modeling* for applications to refinery-like sources and other industrial sources in simple terrain. It is a straight line trajectory, Gaussian-based model that has evolved for over two decades. The most recent version is the ISC3 model, which was based on revisions to the algorithms contained in the ISC2. The ISC3 includes several new features. A revised area source algorithm and revised dry deposition algorithm have been incorporated in the models. The ISC3 also includes an algorithm for modeling impacts of particulate emissions from open pit sources, such as surface coal mines. The ISC Short Term model includes a new wet deposition algorithm, and also incorporates the COMPLEX1 screening model algorithms for use with complex and intermediate terrain.

ISC3 is generally run with a sequence of hourly meteorological conditions to predict concentration at receptors for averaging times of one hour up to a year. In certain cases, hourly data for multiple years are used as inputs to develop a better understanding of the statistics of calculated short-term hourly peaks or longer time averages.

Since the ISC models are especially designed to support the EPA's regulatory modeling programs, the regulatory modeling options, as specified in the Guideline on Air Quality Models (Revised), are the default mode of operation for the models. These options include the use of stack-tip downwash, buoyancy-induced dispersion, final plume rise (except for sources with building downwash), a routine for processing averages when calm winds occur, default values for wind profile exponents and for the vertical potential temperature gradients, and the use of upper bound estimates for super-squat buildings having an influence on the lateral dispersion of the plume. The Short Term model also incorporates the COMPLEX1 screening model dispersion algorithms for receptors in complex terrain, i.e., where the receptor elevation is above the release height of the source. ISC3 allows users to select either rural or urban dispersion parameters, depending on the characteristics of the source location and calculates concentration values or deposition values for a particular run.

The model is capable of handling multiple sources, including point, volume, area, and open pit source types. Line sources may also be modeled as a string of volume sources or as elongated area sources. Several source groups may be specified in a single run, with the source contributions combined for each group. This is particularly useful for Prevention of Significant Deterioration (PSD) applications where combined impacts may be needed for a subset of the modeled background sources that consume increment, while the combined impacts from all background sources (and the permitted source) are needed to demonstrate compliance with the National Ambient Air Quality Standards (NAAQS). The models contain algorithms for modeling the effects of aerodynamic downwash due to nearby buildings on point source emissions, and algorithms for modeling the effects of settling and removal (through dry deposition) of large particulates.

The ISC models have considerable flexibility in the specification of receptor locations. The user has the capability of specifying multiple receptor networks in a single run, and may also mix Cartesian grid receptor networks and polar grid receptor networks in the same run. This is useful for applications where the user may need a coarse grid over the whole modeling domain, but a denser grid in the area of maximum expected impacts.

The major disadvantage of the ISC models is that they do not represent photochemical transformations of trace species. Therefore, it is not possible to represent the conversion of NO to NO_2, HNO_3, and organic nitrates. Moreover, it is not possible to represent the interconversion of gas phase HNO_3 and NH_3 with aerosol phase ammonium nitrate. Because the deposition velocities vary greatly depending on the chemical form of the N species, the ISC models cannot be used to provide reliable estimates of N deposition. At best, the ISC models could be used to estimate upper and lower bounds on N deposition by assuming that all N was in the form of NO (which deposits extremely slowly) or that all N was in the form of HNO_3 which has the most rapid deposition velocity of any N species. The variation in N deposition rates between these two extremes would be so large that the ISC simulations are unlikely to provide any useful information for N deposition estimates.

3.2. AERMOD

The AMS/EPA Regulatory Model (AERMOD) (Cimorelli et al. 1998) is a model developed under the auspices of the AMS/EPA Regulatory Model Improvement Committee (AERMIC) to be a replacement of ISC3 for many applications. It is built upon the framework of ISC3 and retains the single straight line trajectory limitation of ISC3 but contains advanced algorithms to describe turbulent mixing processes in the planetary boundary layer for both convective and stable layers. It also includes a detailed treatment of the dynamics of plumes that rise to interact with elevated inversions at the top of the convective mixed layer.

Since the AERMOD model is especially designed to support the EPA's regulatory modeling programs, the regulatory modeling options are the default mode of operation for the model. These options include the use of stack-tip downwash, and a routine for processing averages when calm winds or missing meteorological data occur. The model also includes non-default options for suppressing the use of stack-tip downwash, and to disable the date checking for non-sequential meteorological data files. The latter option is needed to facilitate evaluation of the model. Currently, the model only calculates concentration values—dry and wet deposition algorithms have not yet been implemented. The user can specify several short-term averages to be calculated in a single run of the AERMOD model, and request the overall period (e.g., annual) averages.

The model is capable of handling multiple sources, including point, volume, and area source types. Line sources may also be modeled as a string of volume sources or as elongated area sources. Several source groups may be specified in a single run, with the source contributions combined for each group. This is particularly useful for PSD applications where combined impacts may be needed for a subset of the modeled background sources that consume increment, while the combined impacts from all background sources (and the permitted source) are needed to demonstrate compliance with the National Ambient Air Quality Standards (NAAQS). The model contains algorithms for modeling the effects of aerodynamic downwash due to nearby buildings on point source emissions. The current version of AERMOD does not include algorithms for modeling depositional effects on particulate emissions.

Source emission rates can be treated as constant throughout the modeling period, or may be varied by month, season, hour-of-day, or other optional periods of variation. These variable emission rate factors may be specified for a single source or for a group of sources. The user may also specify a separate file of hourly emission rates for some or all of the sources included in a particular model run.

The AERMOD model has considerable flexibility in the specification of receptor locations. The user has the capability of specifying multiple receptor networks in a single run, and may also mix Cartesian grid receptor networks and polar grid receptor networks in the same run. This is useful for applications where the user may need a coarse grid over the whole modeling domain, but a denser grid in the area of maximum expected impacts. There is also flexibility in specifying the location of the origin for polar receptors, other than the default origin at (0,0) in x,y, coordinates.

The user can input elevated receptor heights in order to model the effects of terrain above (or below) stack base, and may also specify receptor elevations above ground level to model flagpole receptors. There is no distinction in AERMOD between elevated terrain below release height and terrain above release height, as with earlier regulatory models that distinguished between simple terrain and complex terrain. For applications involving elevated terrain, the user must also input a hill height scale along with the receptor elevation. A terrain preprocessor, called AERMAP, has been developed to facilitate the generation of hill height scales for AERMOD (EPA, 1998c).

AERMOD is similar to the ISC models in that is does not represent chemical partitioning of N between the several gas phase and aerosol components. Therefore, AEROMOD cannot be used to provide meaningful estimates of N deposition rates.

3.3. CALPUFF

CALPUFF (Scire et al. 2000) is a multi-layer, multi-species, non-steady-state, Lagrangian (puff) dispersion model that simulates the effects of time- and space-varying meteorological conditions on pollutant transport, transformation, and removal. It produces predictions of ambient pollutant concentrations, wet deposition fluxes, dry deposition fluxes, and visibility effects such as extinction coefficients. CALPUFF is intended for use on scales from tens of meters to hundreds of kilometers from a source. It includes algorithms for near-field effects such as building downwash, transitional buoyant and momentum plume rise, partial plume penetration, sub-grid scale terrain and coastal interaction effects, and terrain impingement. It also treats longer-range effects such as pollutant removal due to wet scavenging and dry

deposition, chemical transformation, vertical wind shear, over-water transport, plume fumigation, and visibility effects due to PM.

CALPUFF contains a set of computationally efficient puff sampling algorithms that makes its use for simulating long time periods (one or more years) computationally practical. The model can be run in a mode to reproduce the results of straight-line regulatory models such as ISCST3 in steady-state conditions, but CALPUFF offers the advantage of accounting for non-steady state effects when they exist.

CALPUFF includes parameterized gas-phase chemical transformation of SO_2, SO_4, NO, NO_2, HNO_3, NO_3, and organic aerosols. A model for aqueous phase chemical transformation of SO_2 to SO_4 is included. CALPUFF can treat primary pollutants such as PM_{10}, toxic pollutants, ammonia, and other pollutants. The model includes a resistance-based dry deposition model for both gaseous pollutants and PM. Wet deposition is treated using a scavenging coefficient approach. An important limitation of CALPUFF is that the puffs do not recognize in situ values of "background" air concentrations, which will affect the nitrogen partitioning and, hence, the rate of nitrogen deposition.

The model has detailed parameterizations of complex terrain effects, including terrain impingement, side-wall scrapping, and steep-walled terrain influences on lateral plume growth. A gridded field of terrain elevations is used to determine multiple hill effects on plume transport and dispersion. A sub-grid scale complex terrain module based on a dividing streamline concept divides the flow into a lift component traveling over the sub-grid-scale feature and a wrap component traveling around the feature.

Plume dispersion can be treated using turbulence-based dispersion curves. Measured values of turbulence can be used in the model, or estimated values of turbulence will be produced by the model based on similarity theory. There is also an option to use ISCST3 dispersion coefficients (Pasquill-Gifford for rural areas, or McElroy-Pooler for urban areas).

The gridded meteorological fields used by CALPUFF are produced by the CALMET meteorological model. CALMET includes a diagnostic wind field model containing objective analysis and a divergence minimization procedure. Effects such as slope flows, valley flows, terrain blocking, and lake and sea breeze circulations are treated. An energy-balance scheme is used to compute sensible and latent heat fluxes and turbulence parameters over land surfaces. A profile method is used over water. CALMET contains interfaces to prognostic meteorological models such as Versions 4 and 5 of the Penn State/NCAR Mesoscale Model (MM4 and MM5).

Many pre-processor programs are available with the CALPUFF modeling system that allow standard meteorological, terrain, and land use databases to be used directly by the models. Post-processing programs (i.e., PRTMET and CALPOST) provide options for analysis and display of the modeling results. A set of PC-based graphical user interface (GUI) programs can be used to define the model control files.

The chief advantage of CALPUFF is that it achieves computational efficiency by using lookup tables or default concentration fields instead of solving explicitly for VOC-NO_x-Ozone photochemistry. To date there are no published comparisons of CALPUFF to more comprehensive grid models. Therefore, considerable uncertainty remains in the accuracy of CALPUFF for simulating N deposition. The EPA has proposed the use of CALPUFF for applications involving long-range transport over distances beyond 50 km (31 mi). Therefore, it is uncertain whether CALPUFF should be applied for distances of less than 50 km.

3.4. CMAQ PM/Visibility Modeling Systems

The U.S. Environmental Protection Agency developed the CMAQ modeling system to be a one-atmosphere Eulerian air quality modeling system capable of addressing O_3, PM, visibility, and acid deposition within a common three-dimensional platform. CMAQ consists of a core Chemical Transport Model (CTM) and several pre-processors, including the Meteorological-Chemistry Interface Processor (MCIP), initial and boundary conditions processors (ICON and BCON), and a photolysis rates processor (JPROC). EPA is continuing to improve and develop new modules for the CMAQ model and typically provides a new release each year. In the past EPA has also provided patches for CMAQ as errors are discovered and corrected. More recently, EPA has funded the Community Modeling and Analysis Systems (CMAS) center to support the coordination, update, and distribution of the Models-3 system.

The first release of the CMAQ code was in June 1999. When this study was completed the most recent version of CMAQ was the October 2004 release (version 4.4), which is an update to the September 2003 CMAQ Version 4.3 release. This project used the latest publicly available version of CMAQ (v4.4). However, EPA in October 2005 provided a new release of CMAQ, version 4.5. Information on the most current release is available at the CMAQ website: www.cmascenter.org.

The main features of CMAQ for PM modeling are as follows:

- Horizontal and vertical advection.
- Horizontal and vertical diffusion.
- Gas-phase chemistry with the CB-IV, CB-2002, RADM, and SARPC99 mechanisms.
- Aqueous-phase reactions and cloud mixing.
- Modal approach to dynamically represent the PM size distribution using three lognormal modes (2 fine and 1 coarse). Transfer of mass between the aerosol and gas phases is assumed to be in equilibrium. All secondary aerosol (sulfate, nitrate, and secondary organic aerosol (SOA)) is assumed to be in the fine modes.
- The thermodynamics of inorganic aerosol composition are treated using the ISORROPIA module. Aerosol composition is coupled to mass transfer between the aerosol and gas phases.
- Aqueous phase chemistry is simulated using the RADM module. This includes oxidation of SO_2 to sulfate by ozone, hydrogen peroxide, oxygen catalyzed by metals, and radicals. The impact of clouds on the PM size distribution is treated empirically.
- There are four options for treating SOA in CMAQ: the Pandis method, Odum method, Schell method, and SORGAM. The latest is SORGAM, which uses an irreversible semi-volatile scheme whereby VOCs are converted to condensable gases that can then form SOA, but the SOA cannot evaporate back into gases.
- Wet deposition uses the RADM (Regional Acid Deposition Model) approach. Particle dry deposition is included.

4.0 CMAQ and CALPUFF Simulation Results and Discussions

As discussed above, this study's researchers concluded that the simple dispersion models such as ISCT3 and AERMOD cannot be used for modeling N deposition because such models cannot represent the complex chemical and gas-aerosol phase transformations of NO_x and NH_3 in the atmosphere. Because deposition velocities of N species vary dramatically with the chemical form and gas or aerosol state, N deposition models must represent complex photochemical conversions and thermodynamic phase transformations for gas and aerosol species. Therefore, the modeling study of this project focused on the two models that do represent these processes: CMAQ and CALPUFF.

Appendix C describes the CMAQ and CALPUFF model configurations and sources of model-ready input files. The modeling domain shown in Figure 4-1 includes 144 grid cells in the east-west direction and 225 grid cells in the northwest direction. The large north-south dimension was chosen so that the study could simulate hypothetical new power plants in either central or southern California. The east-west domain was chosen to be large enough to include impacts on N-deposition in the Sierra Nevada mountains. This domain is considerably larger than that used in typical ISCT3 or CALPUFF permitting applications because it was important to include the effects of long-range transport of N species.

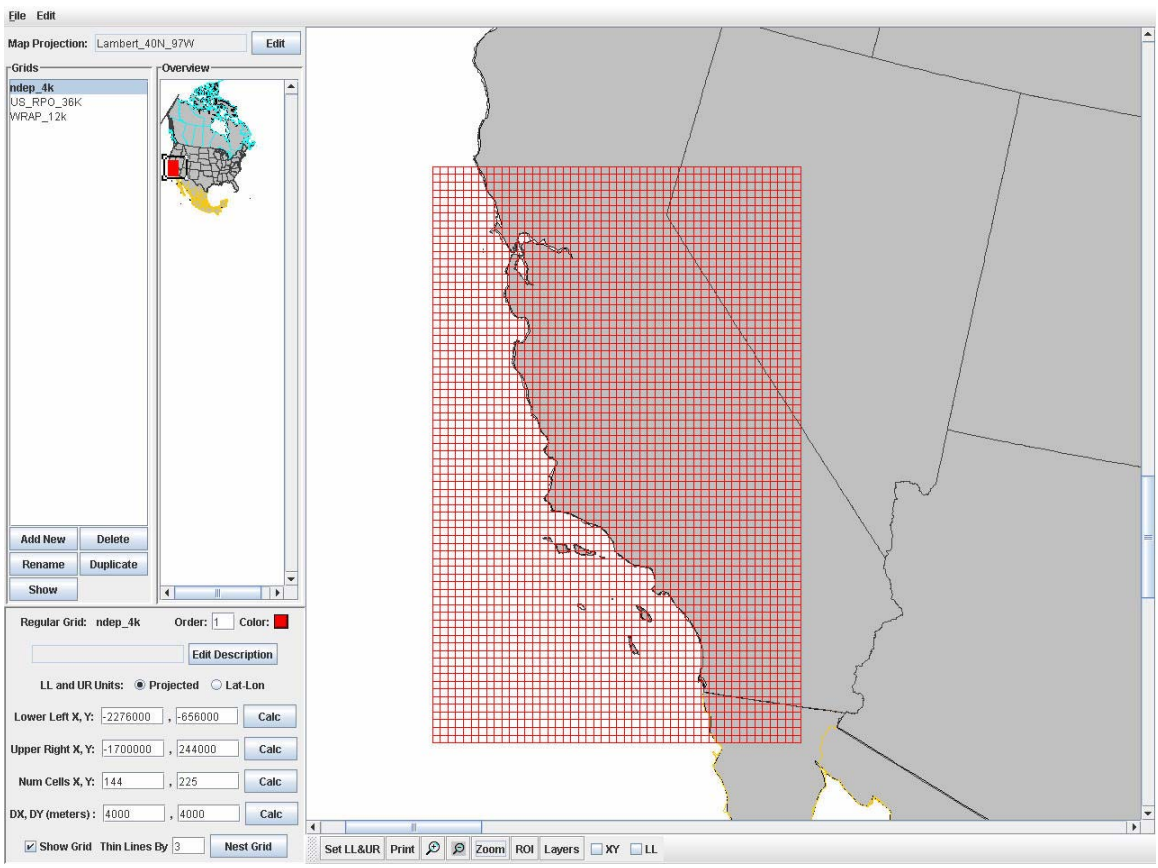


Figure 4-1. 4-km grid resolution modeling domain to be used for the N deposition sensitivity studies in California for both CMAQ and CALPUFF

4.1. CMAQ Results

The CMAQ model was run on the 4-km grid for calendar year 2002 for a "base case" simulation using the actual emissions in 2002. The CMAQ model simulated the emissions, chemical transformations, transport, and deposition of each N species. The total N emissions and N deposition were calculated by integrating over the annual simulation. These results are summarized in Table 4-1.

A total of 7.3×10^8 kilograms (kg) of nitrogen was emitted in the CMAQ modeling domain for the base case simulation, and 26.19% of these emissions were deposited within the modeling domain by the combined dry and wet deposition. Dry deposition accounted for 20.69%, and wet deposition accounted for 5.5% of the total N emissions. Thus, 73.81% of total N emissions were not deposited within the model domain. Most of these emissions would have been transported outside of the domain, while a small portion of the total emissions would have remained in the ambient air within the model domain at the end of the simulation. Because of the prevailing westerly winds in California, it is likely that most of the N was transported out through the eastern boundary of the model domain.

Figure 4-2 shows a spatial map of the annual total N deposition for the CMAQ model 2002 base case for combined dry deposition and wet deposition CMAQ results. All N species were summed when totaling N deposition including HNO_3, NH_3, NO, NO_2, dinitrogen pentoxide (N_2O_5), PAN, and aerosol ammonium nitrate (NH_4NO_3). Figure 4-3 shows the annual total N deposition for the CMAQ 2002 base case for dry deposition and wet deposition. Note that the text at the bottom of each plot identifies the model grid cells in which the minimum and maximum deposition values occurred. For example, in Figure 4-2, the model grid cell with coordinates (92,51) had the maximum deposition rate of 103.6 kg-N/ha/yr. This grid cell included large agricultural operations near Chino in southern California. More detailed analysis of these results showed that the N deposition in this grid cell was mostly dry deposition of NH_3 emitted from the agricultural sources.

After completing the CMAQ base case simulation for the entire year of 2002, CMAQ sensitivity simulations were performed with the Metcalf power station emissions added to the 2002 base case emissions for the months of January and July. Those sensitivity results were compared to the CMAQ base case January and July simulation. These two months were chosen to represent seasonal variations for summer and winter conditions. An annual CMAQ simulation for the sensitivity case was not performed, because of the large computational resources required to complete the annual simulation and because of problematic results in the CMAQ model sensitivity case, as discussed below.

The CMAQ base case monthly total N dry and wet deposition for January and July are shown in Figure 4-4. Table 4-2 summarizes the CMAQ base case emissions, dry and wet deposition, and ratios in January and July, 2002. The modeled dry deposition in July was almost 50% more than in January. This is due to the approximately 50% more emissions released in July than in January. Wet deposition in January was at least an order of magnitude higher than wet deposition in July. CMAQ predicts low wet deposition in July because there is very little precipitation in California in the summer months. However, CMAQ does not represent fog chemistry or deposition by fog, so it is possible that CMAQ underestimates wet deposition in summer months. The southern California region demonstrates the highest level of nitrogen deposition, followed by areas in the San Joaquin Valley. The high levels of nitrogen deposition

in the valley are caused by ammonia emissions from agricultural operations, including animal waste and fertilizer use, with a smaller (but significant) contribution from NO_x emissions.

This study calculated the Metcalf power station impacts on N deposition in the modeling domain by taking the difference between the modeled N deposition in the sensitivity case and the base case. Figure 4-5 shows the change in the monthly total N dry and wet deposition July, and Figure 4-6 shows the change in the monthly total N dry and wet deposition in January. In these plots, yellow to red colors indicated areas in which N deposition increased with the addition of the Metcalf emissions, and blue colors indicate area in which N deposition decreased with the addition of the Metcalf emissions.

The Metcalf emissions added to the sensitivity case were 34,142 kg-N/yr, added in grid cell (26,165). Because the added emissions from the Metcalf power plant were small compared to the total base case N emissions, Figures 4-5 and 4-6 show small changes in N deposition compared to the monthly total base case emissions (shown in Figure 4-4). During July most of the deposition was in the form dry deposition, and the change in N deposition from Metcalf was located close to the power station with a maximum increase of 0.05 kilograms of nitrogen her hectare per month (kg-N/ha/month) in grid cell (26,165). As expected, the change in wet deposition was small because there was very little wet deposition in the base case in summer months. Figure 4-5 does show small increase in wet deposition in the Metcalf sensitivity case with a maximum increase of 0.0001 kg-N/ha/month in grid cell (28,153), i.e., about 55 km (34 mi) south-southeast of the grid cell in which the Metcalf emissions were located. The maximum impact for wet deposition occurs at a greater distance downwind than for dry deposition because incorporation of N into clouds droplets occurs primarily by absorption of secondary N products, and these secondary products are formed from primary emissions of NO_x and NH_3. By contrast, dry deposition occurs most rapidly in the chemical species HNO_3 which is rapidly formed from NO_x emissions during summer months.

Figure 4-6 shows changes in N deposition in the January sensitivity case that appears to result primarily from numerical error in the CMAQ model. For example, the model shows the larges changes in N deposition in southern California even though the emissions were added in the Bay Area. The large area of increased N wet deposition in Southern California in January was clearly not caused by the Metcalf power plant. The pattern of change in the Figure 4-6 wet deposition plot with areas of increases randomly mixed with areas of decrease in N deposition is also indicative of numerical noise.

It is generally known that the CMAQ model is susceptible to numerical noise in the thermodynamics algorithm. However, this numerical noise typically exhibits as isolated grid cells with random increases or decreases in the concentrations of aerosol species. In previous CMAQ air quality simulations, this study's researchers routinely performed emissions reduction sensitivity runs and did not observe widespread, systematic numerical noise like that seen in Figure 4-6 in southern California. Because the results were contrary to what was expected, several tests and quality control checks were performed to verify that no errors had been made with the simulations.

First, researchers verified that that the only difference between the base case and sensitivity case emissions was from the Metcalf power plant. The researchers first noted the problem with numerical noise in CMAQ version 4.3. Then, researchers repeated the model simulations using an updated version of CMAQ 4.4 and were able to reproduce the numerical errors using the updated version of the CMAQ model. Finally, researchers ran the base case and sensitivity case

over, but turned off the aerosol routines. By not running aerosol, researchers were able to eliminate the numerical noise in the Southern California region. These tests confirm that the source of the numerical noise in the January simulations is the aerosol thermodynamics algorithm in the CMAQ model.

Based upon the findings, the aerosol routines in the CMAQ version 4.4 air quality model may not be suitable currently to handle nitrogen deposition from single source. The authors recommend testing another air quality model, either an updated version of CMAQ or ENVIRON Corporation's CAMx photochemical grid model, to see if it is better able to simulate the effects of adding a single emissions source.

Table 4-1. Summary of total 2002 base case domain-wide emissions; dry, wet, and combined deposition; and ratios for 2002 CMAQ base case

	Annual domain-wide Emissions (kg-N/year)	Annual Deposition (kg-N/year)	% (annual depo/emis)
Dry	7.31e+8	1.51e+8	20.69 %
Wet		0.40e+8	5.50 %
Total		1.92e+8	26.19 %

Table 4-2. Summary of CMAQ Base Case emissions, dry and wet deposition, and ratios in January and July

	% of annual domain-wide emissions	Emissions (kg-N/month)	Dry Deposition (kg-N/month)	Wet Deposition (kg-N/month)	% (depo/emis)	
					Dry	Wet
January	7.44	5.44e+7	7.88e+6	5.71e+6	14.5	10.5
July	9.62	7.03e+7	1.80e+10	5.15e+5	25.6	0.7

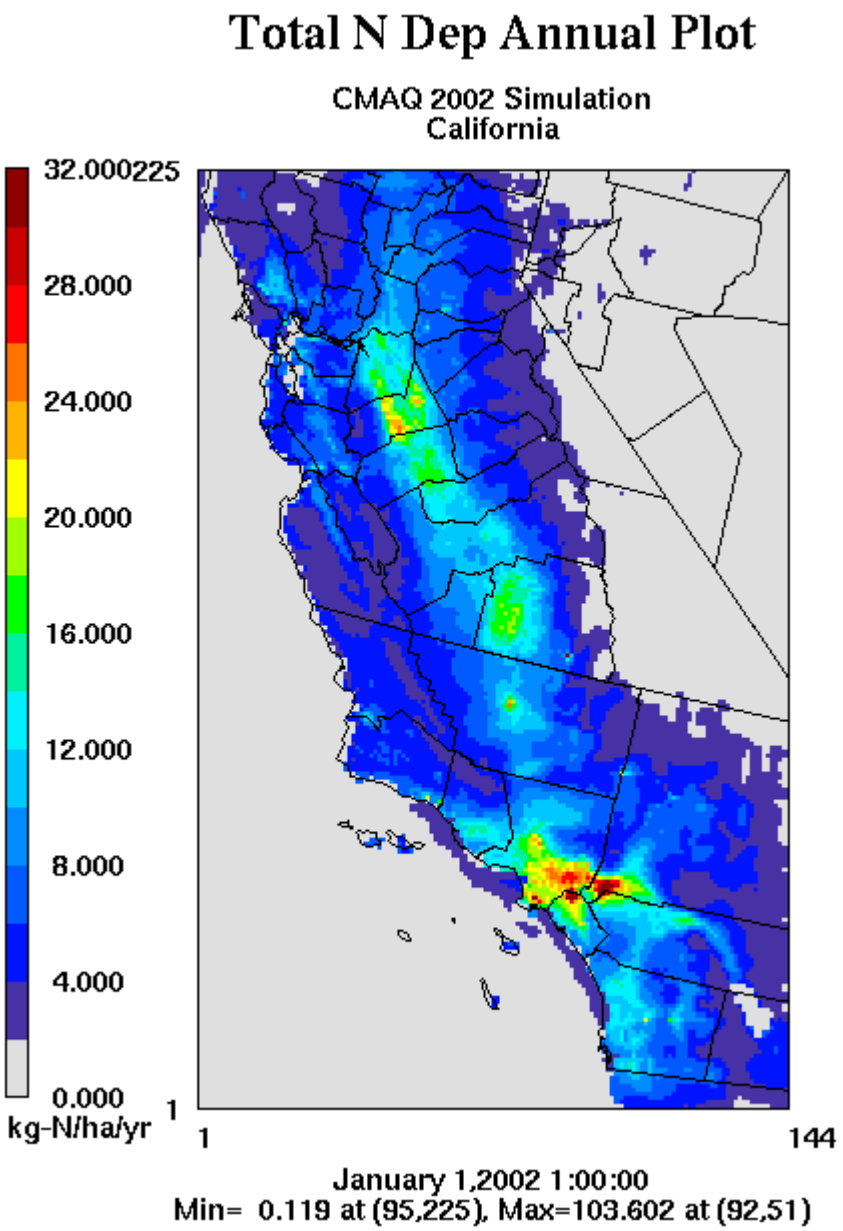


Figure 4-2. Annual total N deposition for the CMAQ air quality model 2002 base case for combined dry deposition and wet deposition

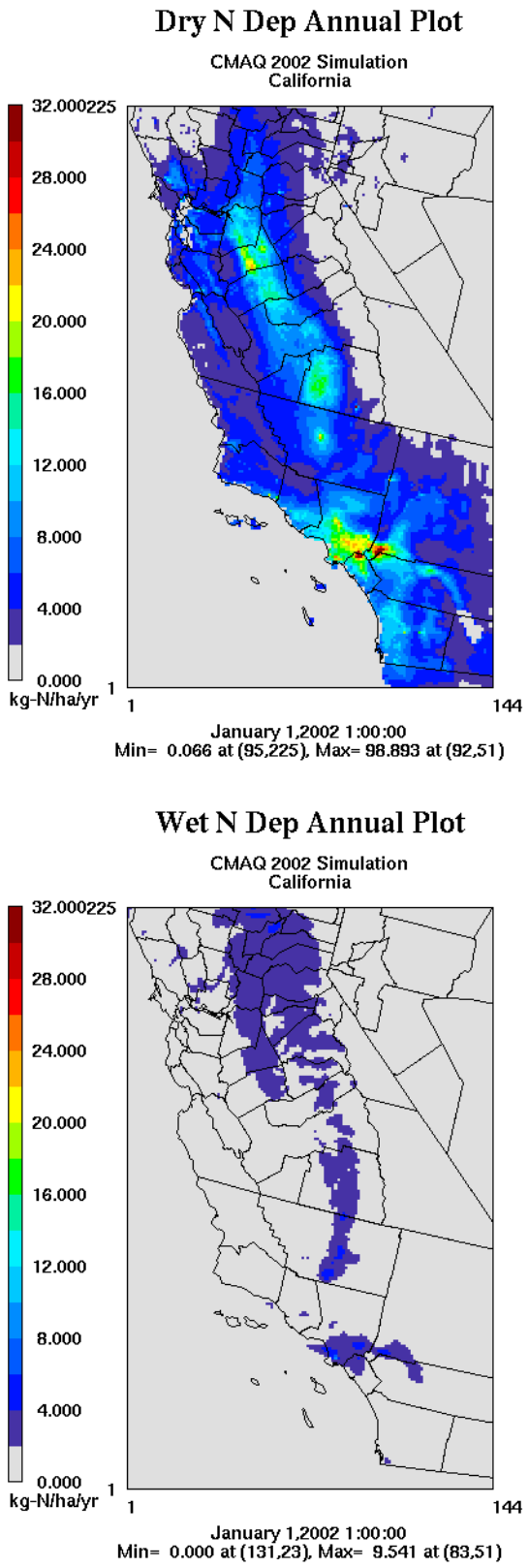


Figure 4-3. Annual total N deposition for the CMAQ air quality model 2002 base case for: (top) dry deposition; and (bottom) wet deposition

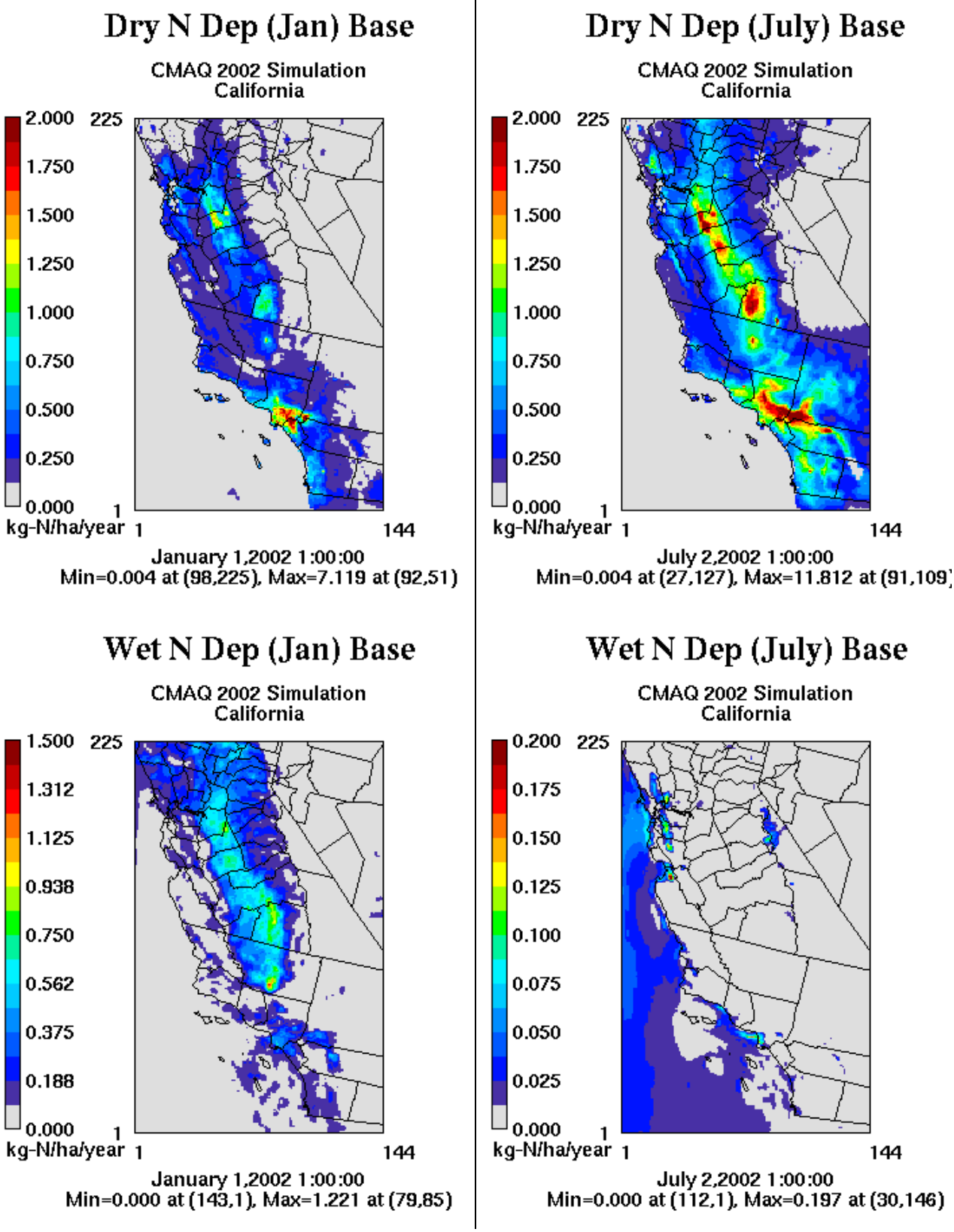
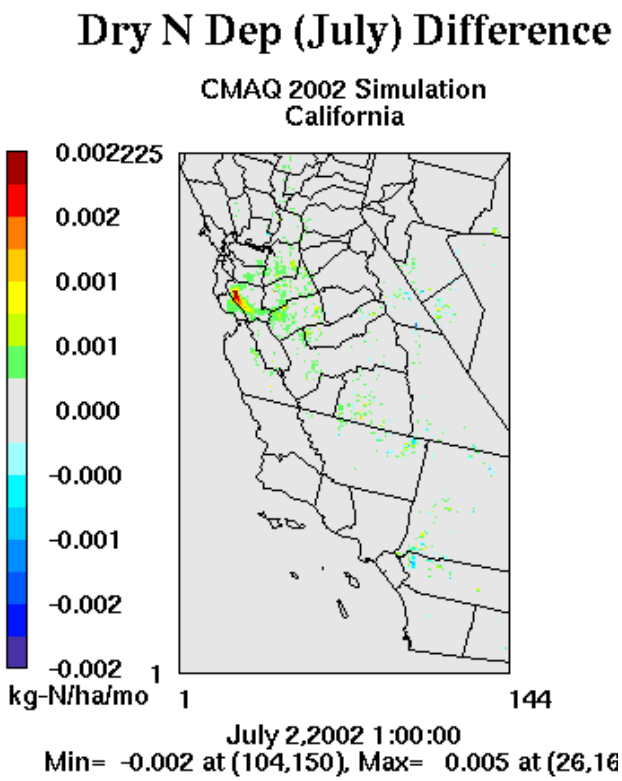


Figure 4-4. CMAQ base case January and July N deposition: dry deposition (top); and wet deposition (bottom). Note different scales in wet deposition plots.



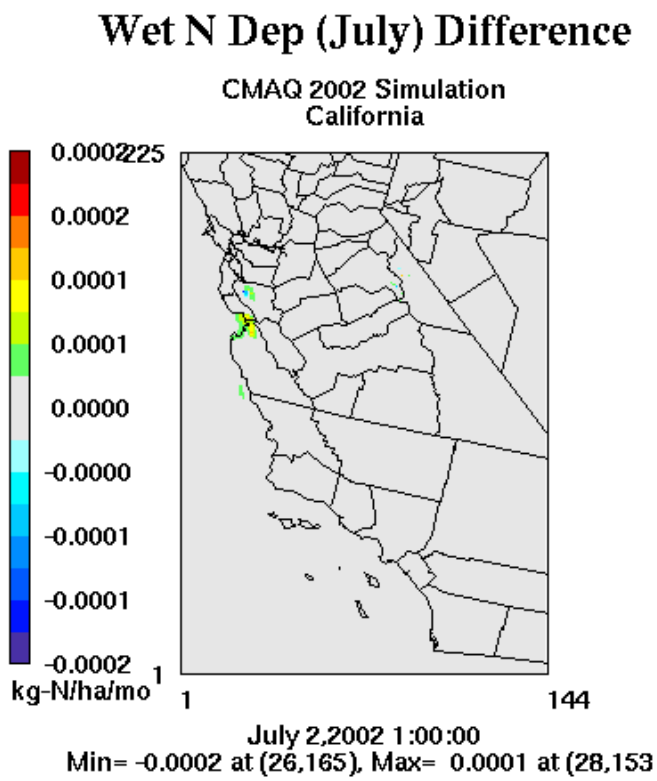
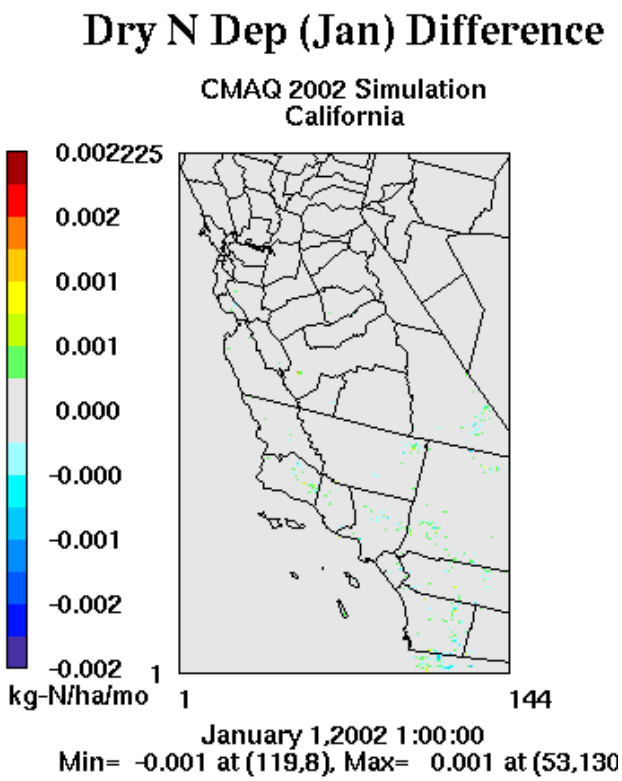


Figure 4-5. CMAQ monthly N deposition difference during July between the sensitivity case and base case for dry deposition (top plot) and wet deposition (bottom plot). Note that there is a 10x difference in scale between the two plots.



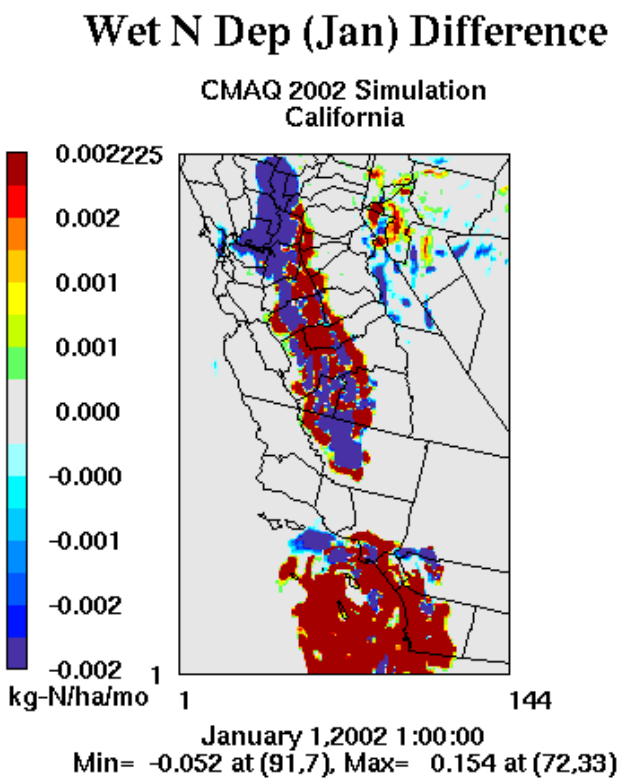


Figure 4-6. CMAQ monthly total N wet deposition difference between sensitivity case and base case for January (top plot) and July (bottom plot)

4.2. CALPUFF Results

A description of the CALPUFF model is included above in Section 3.3. The results presented here are from 2002 January and July CALPUFF simulations using the same model domain used in the CMAQ modeling (shown in Figure 4-1). Because the CALPUFF model uses individual air parcels or "puffs" to represent each emissions source, it is not well suited for modeling large numbers of emissions sources from a variety of emissions source categories. Moreover, it is not well suited for simulating the interactions of air parcels and therefore cannot represent the interaction of multiple emissions sources. Instead, CALPUFF specifies background concentrations of key pollutants and then simulates the chemical transformations of a particular emissions source as it interacts with the background concentration. While it is possible to operate CALPUFF by reading in time and space varying concentration fields developed from a photochemical grid model such as CMAQ, this would require considerable effort and was beyond the scope of this study. Therefore, default background concentrations were used as input to the CALPUFF model.

Because CALPUFF does not represent all emissions sources, it cannot be used to develop N deposition estimates for a base case scenario similar to that presented in the CMAQ results in Section 4.1. Instead, this study's researchers operated CALPUFF to represent NO_x emissions from the Metcalf power plant, including their chemical transformations as they interacted with background O_3 and NH_3, and to calculate the amount of N deposition that could be directly attributed to Metcalf NO_x emissions.

The meteorological inputs were processed by CALMM5/CALMET from the same set of MM5 results used in the CMAQ model. In the "CALPUFF.INP" file used to specify the model setup, the Metcalf power plant emissions were released as a point source. Table 4-3 shows the total amount of emissions released in the two months, the amount of dry and wet deposition in the modeling domain, and the percentage of emissions deposited. The researchers set up the CALPUFF model simulation so that the total amount of emissions was identical to that released from the Metcalf power plant in the CMAQ model simulations. The monthly emissions rate varies as follows: 6.89% of the annual emissions were released in January; and 10.18% of annual emissions were released in July. In January, approximately 9.8% of total N emissions was deposited in the model domain by dry deposition while 1.5% was deposited by wet deposition. In July, 24.8% of the total N emissions was deposited by dry deposition and 0.4% was deposited by wet deposition.

Although Table 4-3 shows the percentage of the Metcalf N emissions that deposited within the model domain, these results cannot be directly compared to CMAQ results in Table 4-2 because the CMAQ results were based on the amount of N deposited from the total emissions inventory, not from a single point source. It is also difficult to specify what percentage of the CMAQ Metcalf emissions deposited within the model domain because of the large numerical noise in the CMAQ aerosol thermodynamics algorithm. With that caveat, it is possible to compare the percentage of the CALPUF Metcalf N emissions that deposited (shown in Table 4-3) versus the percentage of the CMAQ total N emissions that deposited within the model domain (shown in Table 4-2). In January for the CALPUFF model 11.3% of N emissions deposited compared to 25.0% of all N emissions sources in the CMAQ model, and in July 25.2% of the Metcalf N emissions deposited compared to 26.3% of all N emissions sources in CMAQ.

Table 4-3. Summary of CALPUFF total emissions, dry deposition, and ratios in January and July, 2002

	% of annual Metcalf Emissions	Emissions (kg-N/month)	Dry Deposition (kg-N/month)	Wet Deposition (kg-N/month)	% (depo/emis)	
					Dry	Wet
January	6.89	3472.36	340.68	53.04	9.8	1.5
July	10.18	5133.05	127.33	18.55	24.8	0.4

Figure 4-7 shows the CALPUFF monthly total N dry deposition from the Metcalf power plant for July. In this plot, the scale ranges from -0.001 to 0.001 kg-N/ha/mo, to better indicate the extent of the area of N deposition; while all other CALPUFF plots in this report use a scale from -0.002 to 0.002 kg-N/ha/mo, to better indicate the area of maximum deposition. The CALPUFF results show that most of the deposition occurred close to the Metcalf power plant. The CALPUFF results did not exhibit any numerical noise in Southern California.

Figure 4-8 and 4-9 show the monthly total dry and wet nitrogen deposition from January and July. The results show that both the higher emissions rates in July and meteorology lead to higher deposition values in a larger region within the modeling domain. Similar to the CMAQ results, in CALPUFF dry deposition was considerably larger than the wet deposition.

Appendix C presents more detailed results for the CMAQ and CALPUFF simulation, including a series of plots that show the evolution over time of the hourly N deposition from the Metcalf source as simulated by both models. The CMAQ plots show much more detailed resolution of the spatial variability in N deposition, while the CALPUFF plots show very coarsely resolved areas of N deposition. However, the CMAQ results also show relatively large numerical noise. At some time steps the CALPUFF plots in Appendix C seem to indicate counterintuitive results, with "hot spots" of N deposition occurring at large distances away from the emissions source area. It is possible that this result from pollutants being transported long distances in the upper layers of the model, and then being mixed back down to the surface and deposited. However, another modeling study (Boo et al. 2005) has also shown counter-intuitive results in CALPUFF with hot-spots of sulfate concentration at long distances downwind of the source area. This is shown in Figure 4-10 (from Boo et al. 2005) in which SO_X emissions in Chicago produce high sulfate concentration in the Chicago area and also in a hot spot off the coast of Massachusetts. Further investigation of these results is required before the CALPUFF model can be used with confidence in N deposition modeling.

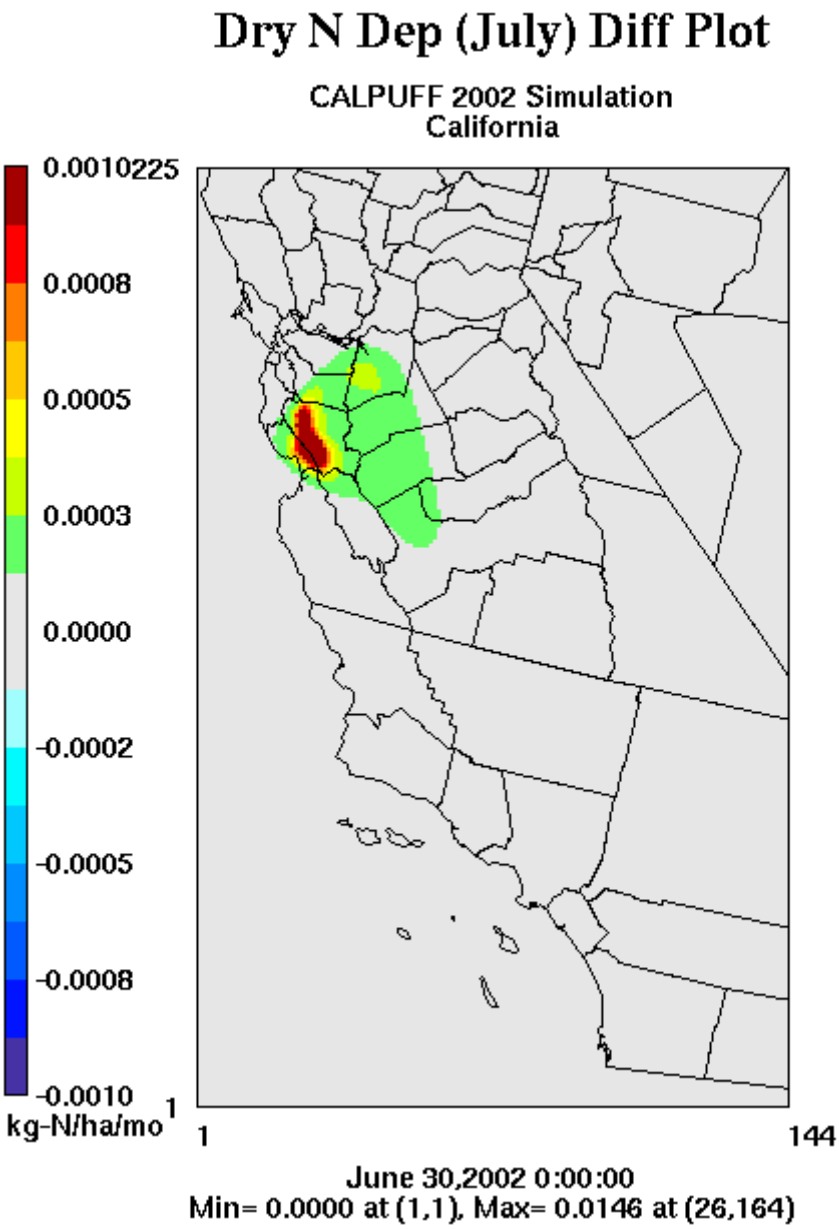
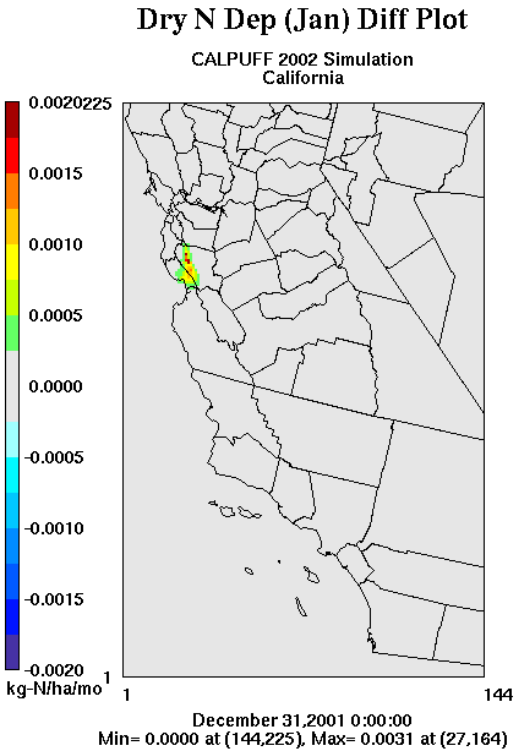


Figure 4-7. CALPUFF model simulated July total N dry deposition for the Metcalf power plant. (Note that the scale in this plot is from -0.001 to 0.001 kg-N/ha/mo)



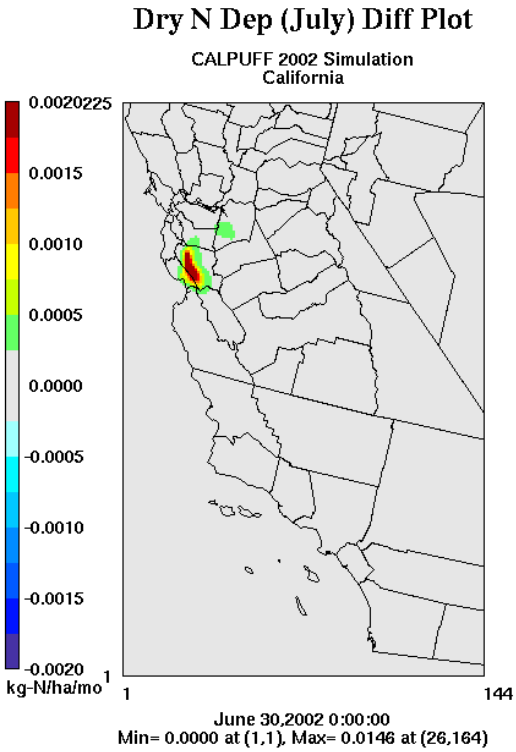
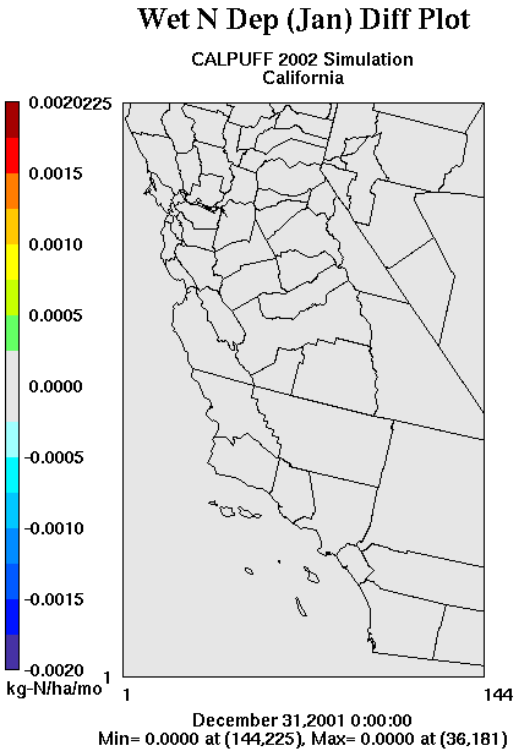


Figure 4-8. CALPUFF model simulated monthly total N dry deposition for January (top) and July (bottom) for the Metcalf power plant



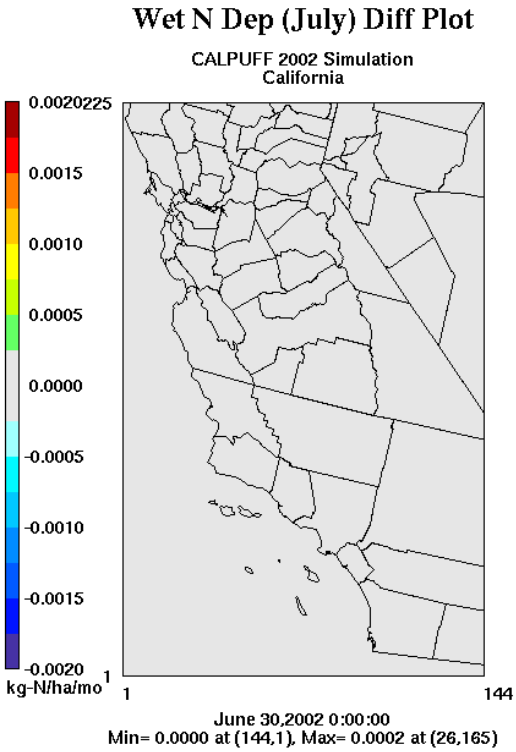


Figure 4-9. CALPUFF model simulated monthly total N wet deposition for January (top) and July (bottom) for the Metcalf power plant

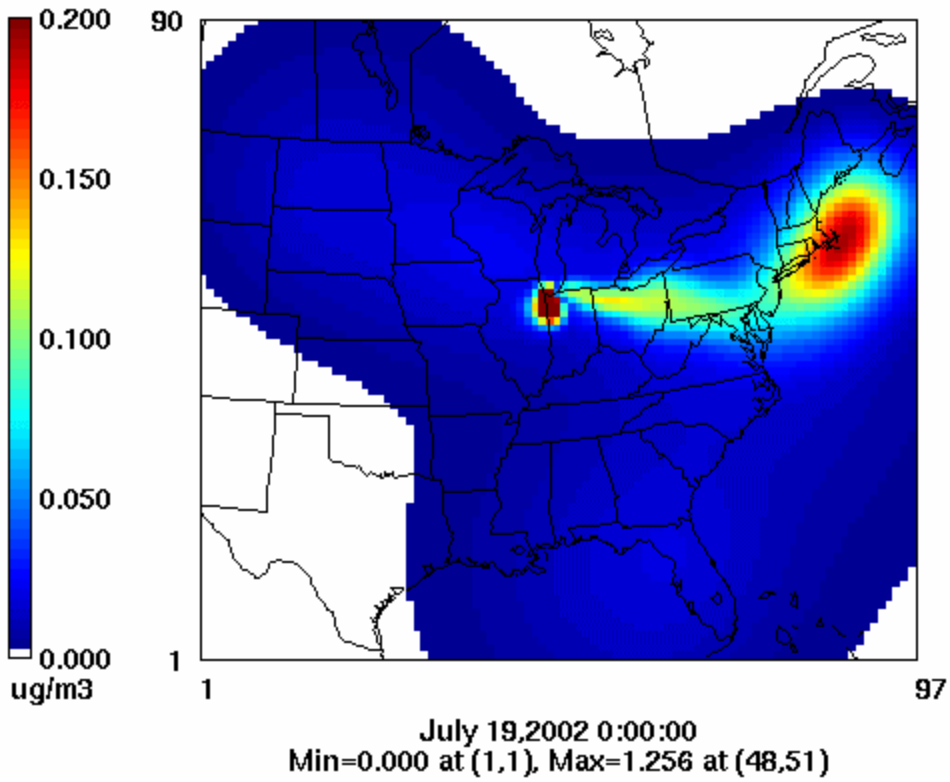


Figure 4-10. Results from CALPUFF modeling of ambient sulfate concentrations in a separate study performed by ENVIRON Corporation, in which CALPUFF appears to exhibit an artifact of a high concentration spike at significant distances downwind of the source area (figure provided by ENVIRON Corporation).

5.0 Transfer of CMAQ Model Datasets

To transfer the CMAQ air quality model results to other researchers, the deposition values were converted from standard CMAQ binary format into an ASCII file. Researchers then used Arc Toolbox to convert the ASCII values into raster. The next step was to define the Lambert Conformal Projection based on the CMAQ modeling domain.

Next, researchers used the corner of the raster to align the maps and manually georeference the raster to the nitrogen deposition CMAQ air quality modeling domain, as shown in Figure 5-1. Finally, researchers were then able to overlay the dry nitrogen deposition from the CMAQ air quality model over the map of Southern California region, as shown in Figure 5-2. The datasets for the annual CMAQ nitrogen deposition have been transferred to other study participants and to researchers at the University of California Center for Conservation Biology, and are available to others upon request.

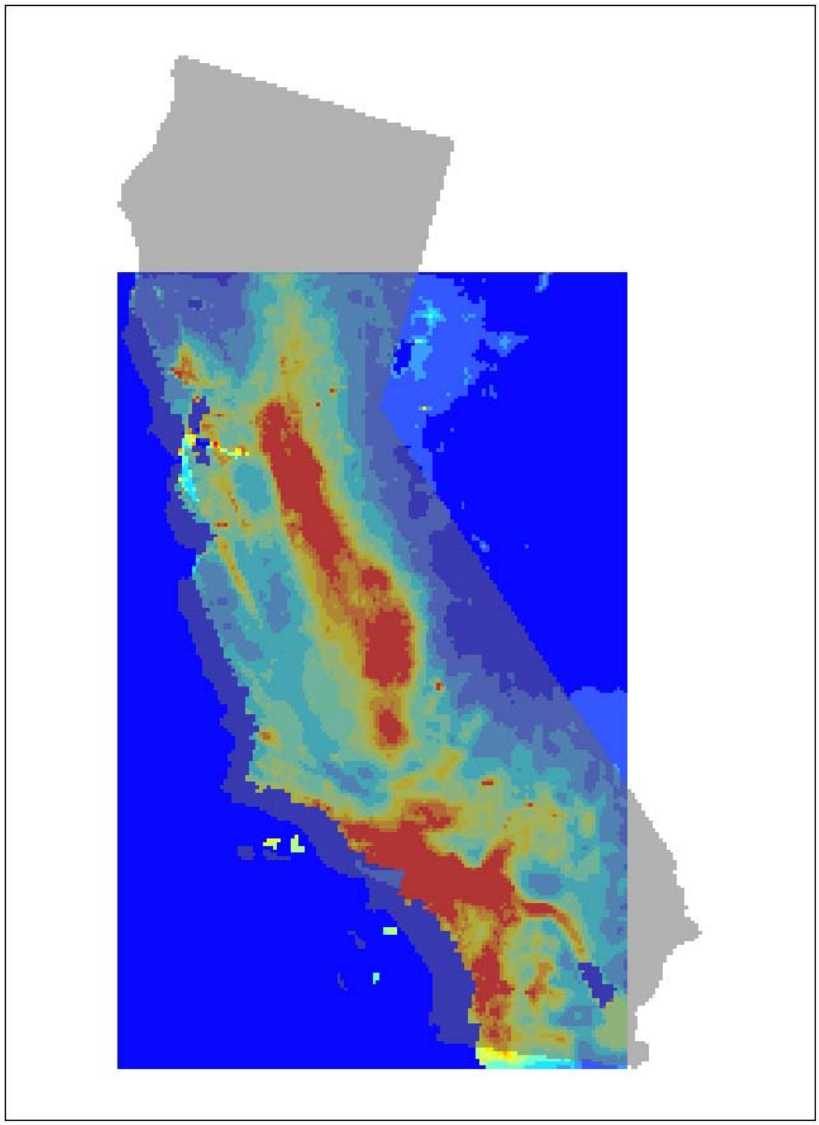


Figure 5-1. Mapping the raster data to the modeling domain

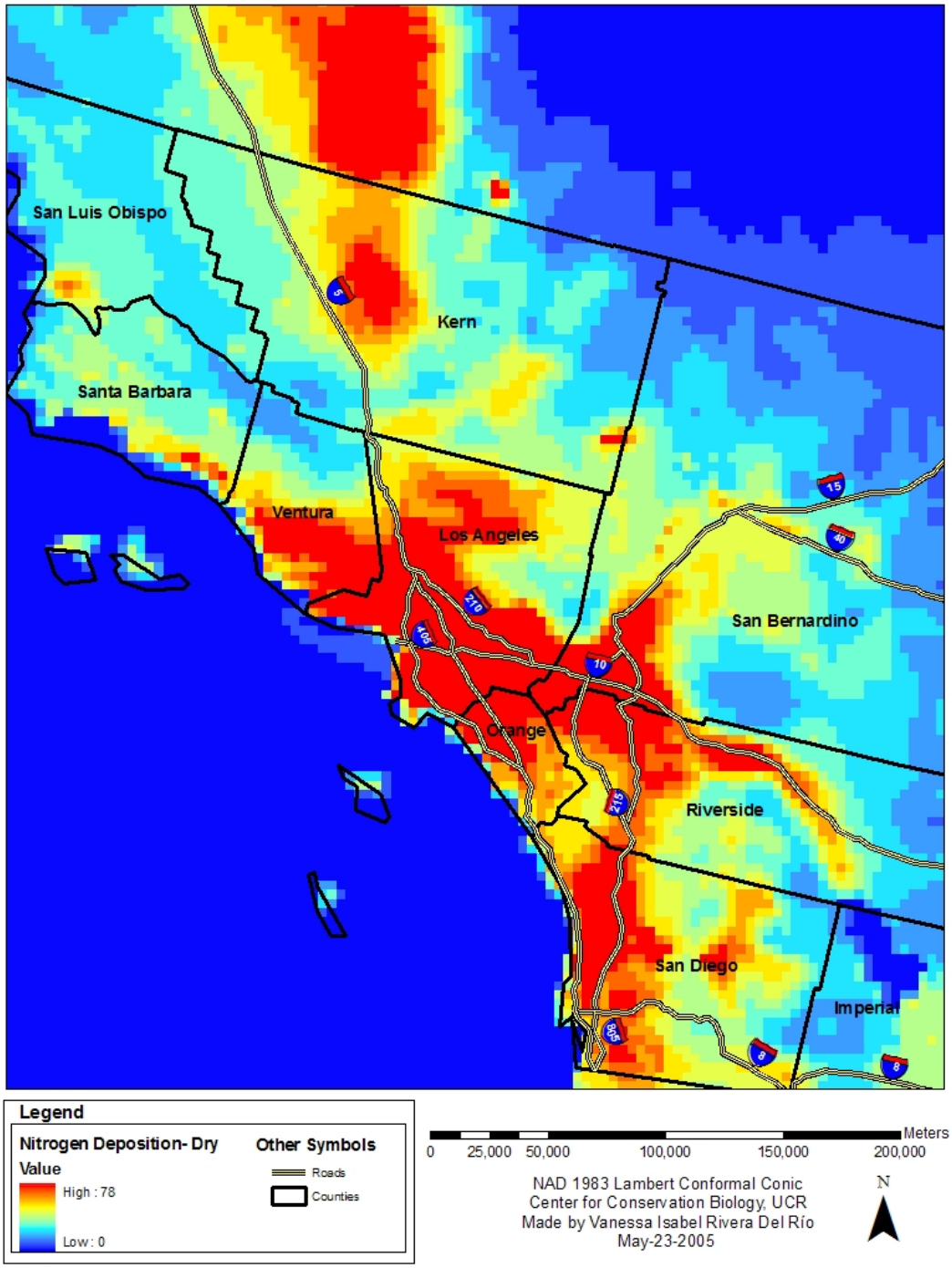


Figure 5-2. Dry nitrogen deposition simulated by the CMAQ model in Southern California

6.0 Conclusions and Recommendations

This study reviewed four air quality models that are widely used for air quality modeling studies. The authors concluded that the simple Gaussian dispersion models—ISCT3 and AERMOD—are not suitable for modeling N deposition, because they fail to represent chemical and phase transformation of the NO_X and NH_3 emissions. Because the deposition velocity and also uptake by clouds is highly dependent on the chemical form and also the state (i.e., gas or aerosol), an air quality model must be designed to represent speciation and aerosol thermodynamics to simulate accurately N deposition. Thus, this study did not pursue any additional modeling using the ISC and AERMOD models, and the authors do not recommend these for use in N deposition studies.

This study also reviewed two models that showed some promise for N deposition assessments: the CALPUFF trajectory model and the CMAQ photochemical grid model.

As shown in Figures 4-6, CMAQ sometime produced relatively large numerical error for sensitivity applications using small changes to the base emissions inventory. Typically the errors in sensitivity applications manifest as random errors in isolated grid cells. In the NO_x point source simulation used in this project, the errors manifested more uniformly and over a large number of grid cells in Southern California. Presumably this is a modeling artifact that results from the CMAQ ISORROPIA aerosol algorithms; however, this research was unable to fully explain the causes of this error. As a result of this error it appears that CMAQ cannot be used reliably for single point source sensitivity simulations. It is possible that other Eulerian photochemical grid models that use the ISORROPIA algorithms may also demonstrate similar problem, although testing would need to be completed to verify this possibility. Alternatively, new source apportionment algorithms currently being implemented in CMAQ and CAMx could be used to track the N deposition from individual point sources. Work in this area is currently in progress at UCR for the CMAQ model and at ENVIRON Corporation for the CAMx model.

CALPUFF simulations do not suffer from the same numerical errors as those observed in the CMAQ modeling. However, there is still concern regarding the CALPUFF modeling because of the "hot spots" that occur at significant distances downwind of the emissions point source. It is possible that these hot spots result from upper level emissions that are advected downwind and then mixed to surface; however, the spatial distribution of the deposition hot spots in this work seems counterintuitive and requires further investigation. As discussed in Section 4 and illustrated in Figure 4-10, other applications of the CALPUFF model also show counterintuitive results with high ambient concentration of sulfate at significant distances from the point source. Moreover, there are important concerns regarding the formulation of the CALPUFF model. The sulfate and nitrate chemistry used in CALPUFF was developed in 1983 and is now out-of-date and inaccurate. Because CALPUFF used background O_3 (instead of simulating photochemical O_3 formation) it also fails to account for the effects of NO_X on oxidant limiting conditions for sulfate formation.

Thus, uncertainty remains in the CALPUFF modeling results, and further research is needed to test the reliability of these results. Comparisons with future CAMx and CMAQ simulations using the source apportionment algorithms should be useful to investigate these concerns.

In the January 2002 scenario, dry and wet deposition accounted for 14.5% and 10.5% of the CMAQ base case N deposited, respectively. In the July 2002 scenario, 25.6% and 0.7% of CMAQ base case N deposition are from dry and wet deposition, respectively. Although the deposition rates are for the CMAQ domain-wide base case dry and wet deposition, these values may be, under certain circumstances, similar to the rates applied to the Metcalf power plant's emissions if no numerical error existed in the CMAQ air quality model. From the CALPUFF results, January dry and wet deposition rate from the Metcalf power plant are 9.8% and 1.5%, respectively. In July, the dry and wet deposition rates are 24.8% and 0.4%, respectively.

For both CMAQ and CALPUFF air quality models, dry deposition rates are consistently higher than wet deposition rates. The rates of dry and wet deposition from the CMAQ air quality model in January tend to be higher than the CALPUFF model. It is possible that in the CMAQ base case, areas of precipitation away from the direct influence of Metcalf power plant contributed to the removal of N emissions, which led to the higher wet deposition rates. In this project's CALPUFF simulations, wet deposition of nitrogen occurs only in the regions that are influenced by Metcalf power plant. In July, dry and wet deposition magnitudes are comparable for both CMAQ and CALPUFF. This evidence also suggests that future model inter-comparison studies on nitrogen deposition should further examine wet deposition in California in winter months.

7.0 References

Ames, R. B., and W. C. Malm. 2001. "Comparison of sulfate and nitrate particle mass concentrations measured by IMPROVE and the CDN." *Atmospheric Environment* 35: 905–916.

B. Koo, S. Lau, A. Hoats, G. S. Tonnesen, C. J. Chien, and Z. S. Wang. 2005 "Alternative Model Simulations: CAMx vs. CMAQ and PSAT vs. TSSA." WRAP Modeling Forum Meeting, San Francisco, California.

Byun, D. W., and J. K. S. Ching. 1999. "Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System." EPA/600/R-99/030.

Byun, D., 1999a. "Dynamically consistent formulations in meteorological and air quality models. Part I: Governing equations in a generalized coordinate system." *J. Atmos. Sci. 56* 3787–3807.

Byun, D., 1999b. "Dynamically consistent formulations in meteorological and air quality models. Part I: Mass conservation issues." *J. Atmos. Sci.* 56: 3808–3820.

CEP. 2004. *SMOKE Users Manual*. Houyoux, M., Vukovich, J., and Brandmeyer, J.E., Carolina Environmental Program, University of North Carolina, Chapel Hill, North Carolina, 27516.

Cimorelli A. J., S. G. Perry, A. Venkatram, J. C. Weil, R. J. Paine, R. J. Wilson, R. F. Lee, and W. D. Peters. 1998. AERMOD-–Description of Model Formulation (Version 98314 (AERMOD and AERMET) and 98022 (AERMAP). USEPA, RTP, NC 27711, 113 pages.

Dennis, R. L., D. W. Byun, J. H. Novak, K. J. Galluppi, C. J. Coats, and M. A. Vouk. 1996: The next generation of integrated air quality modeling: EPA's Models-3. *Atmospheric Environment* 30:(12) 1925–1938.

Fenn, M. E., R. Haebuer, G. S. Tonnesen, J. S. Baron, S. Grossman-Clarke, D. Hope, D. A. Jaffe, S. Copeland, L. Geiser, H. M. Rueth, and J. O. Sickman. 2003. "Nitrogen Emissions, Deposition and Monitoring in the Western United States." *BioScience* 53: 391–403.

Fenn, M. E., J. O. Sickman, A. Bytnerowicz, D. W. Clow, N. P. Molotch, J. E. Pleim, G. S. Tonnesen, K. C. Weathers, P. E. Padgett, and D. H. Campbell. 2005. "Methods for Measuring Atmospheric Nitrogen Deposition Inputs in Arid and Montane Ecosystems of Western North America." Manuscript submitted to the Developments in Environmental Science series, Elsevier Press, submitted 11/18/05.

Grell, A. G., J. Dudhia, and D. R. Stauffer. 1994. A description of the fifth generation Penn State/NCAR mesoscale model (MM5). NCAR Technical Note NCAR/TN 398+STR, National Center for Atmospheric Research, Boulder, Colorado.

Kembell-Cook S., Y. Jia, C. Emery, R. Morris, Z. S. Wang, G. S. Tonnesen. 2005. "Draft Final Report, Annual 2002 MM5 Meteorological Modeling to Support Regional Haze Modeling of the Western United States." Prepared for The Western Regional Air Partnership, 1515 Cleveland Place, Suite 200, Denver, Colorado, 80202.

Morris R. E., G. Yarwood, B. Koo, S. Lau, A. Hoats, G. S. Tonnesen, C. J. Chien, and Z. S. Wang. 2005 "Alternative Model Simulations: CAMx vs. CMAQ and PSAT vs. TSSA." WRAP Modeling Forum Meeting, San Francisco, California.

Pleim, J. E., and J. S. Chang. 1992. A non-local closure model for vertical mixing in the convective boundary layer. *Atmospheric Environment* **26A** 965–981.

Reisner, J., R. M. Rasmussen, and R. T. Bruintjes. 1998. "Explicit forecasting of supercooled liquid water in winter storms using the MM5 mesoscale model." *Quart. J. Roy. Metero. Soc.*124 B, 1071–1107.

Scire J. S., D. G. Strimaitis, and B. J. Yamartino. 2000. *A User's Guide for the CALPUFF Dispersion Model (Version 5).* Earth Tech, Inc.: Concord.

Seigneur C., B. Pun, P. Pai, J. F. Louis, P. Solomon, C. Emery, R. Morris, M. Zahniser, D. Worsnop, P. Koutrakis, W. White, and I. Tombach. 2000. "Guidance for the Performance Evaluation of Three-Dimensional Air Quality Modeling Systems for Particulate Matter and Visibility." *JAWMA* 50: 588–599.

Stauffer, D. R., and N.L. Seaman. 1990. "Use of Four-Dimensional Data Assimilation in a Limited-Area Mesoscale Model. Part I: Experiments with Synoptic-Scale Data." *Monthly Weather Review* 118(6): 1250–1277.

Stauffer, D. R., N. L. Seaman, and F. S. Binkowski. 1991. "Use of Four-Dimensional Data Assimilation in a Limited-Area Mesoscale Model. Part I: Effects of Data Assimilation within the Planetary Boundary Layer." *Monthly Weather Review* 119(3): 734–754.

Tonnesen, G. S., Z. S. Wang, M. Omary, C. J. Chien, B. Wang. 2003a. Central California Ozone Study (CCOS) 2000 Model Intercomparison for SAQM, CMAQ and CAMx with CB4 and SAPRC99. Presentation to the California Air Resources Board. January 27.

Tonnesen, G. S., Z. Wang, M. Omary, Y. Qin, M. Chitjian. 2003b. Modeling Air Quality Effects of NO_X and PM Emissions from Backup Diesel Generators. Report to the California Energy Commission, Sacramento, California, February 13, 2003.

Tonnesen, G. S., Z. Wang, M. Omary, C. J. Chien, B. Wang, R. Morris, M. Houyoux, Z. Adelman, and U. Shankar. 2002. WRAP Regional Haze CMAQ 1996 Model Performance Evaluation. The WRAP Section 309 SIP Coordination Meeting, Denver, Colorado, July 10, 2002.

Xiu, A., and J. E. Pleim. 2000. "Development of a land surface model. Part I: Application in a mesoscale meteorology model." *Journal of Applied Meteorology* 40: 192–209.

8.0 Glossary

AGL	above ground level
AIRMoN	Atmospheric Integrated Research Monitoring Network
AIRS	Aeronomic Information Retrieval System
API	Application Programming Interface
AQS	U.S. EPA's Air Quality System
ArcInfo	A comprehensive GIS for data management, visualization, modeling, and analysis
BCON	An initial and boundary conditions processor
BEIS	Biogenic Emission Inventory System
CALMET	A diagnostic three-dimensional meteorological model
CALMM5	An interface program that extracts and interprets output data from MM5
CALPOST	A post-processing program
CALPUFF	air quality dispersion model
CAMx	Comprehensive Air quality Model with extensions
CASTNET	Clean Air Status and Trends Network
CB-2002	Carbon Bond mechanism (2002)
CCOS	Central California Ozone Study
CCTM	CMAQ Chemical Tracer Model
CM	coarse matter
CMAQ	U.S. EPA's Models-3 Community Multiscale Air Quality modeling system
CMAS	Community Modeling and Analysis Systems
CTM	Chemical Transport Model
EPA	U.S. Environmental Protection Agency
FM	fine matter
GMT	Greenwich Mean Time
GUI	graphical user interface
HNO_3	nitric acid
ICON	An initial and boundary conditions processor
IDNR	Illinois Department of Natural Resources
IMPROVE	Interagency Monitoring of Protected Visual Environments
I/O	Input/Output
ISCST3	Industrial Source Complex Short Term (ISCST3) model
ISOP	isoprene
ISORROPIA	Aerosol thermodynamic model
JPROC	A photolysis rates processor
LADCO	Lake Michigan Air Directors Consortium
MCIP	Meteorological-Chemistry Interface Processor
MDN	Mercury Deposition Network
MM5	Penn State Mesoscale Model
NADP	National Atmospheric Deposition Program
NADP/NTN	National Atmospheric Deposition Program/National Trends Network
NAMS	National Air Monitoring Stations
NCAR	National Center for Atmospheric Research
NCEP	National Centers for Environmental Prediction

NO	nitric oxide
NO_x	nitrogen oxides
NO_2	nitrogen dioxide
NH_3	ammonia
PAMS	Photochemical Assessment Monitoring Stations
PAN	peroxyacetyl nitrates
PRTMET	A post-processing program
PST	Pacific Standard Time
QA	Quality Assurance
QAPP	Quality Assurance Project Plan
QC	Quality Control
RADM	A random-walk model for simulation of dispersion processes in turbulent fluids
RADM/RPM	A Regional Particulate Model
RAMS	Regional Atmospheric Modeling System
REMSAD	Regulatory Modeling System for Aerosols and Deposition
RNO_3	organic nitrates
RPOs	Regional Planning Organizations
SARPC99	California Statewide Air Pollution Research Center mechanism (1999)
SEARCH	Southeastern Aerosol Research and Characterization
SLAMS	State and Local Air Monitoring Stations
SMOKE	Sparse Matrix Operator Kernel
SOA	secondary organic aerosols
SORGAM	An aerosol module
STN	EPA Speciation Trends Network
UCR	University of California, Riverside
TOMS	Total Ozone Mapping Spectrometer
UNC-CEP	University of North Carolina, Carolina Environmental Programs
USGS	United States Geological Survey
UTC	Coordinated Universal Time
VISTAS	Visibility Improvement State and Tribal Association of the Southeast
VOC	volatile organic compounds
WRAP	Western Regional Air Partnership

Appendix A

Description Meteorology Modeling

1 Meteorological Inputs

New 2002 annual 4 km meteorological data needed to be developed for this project. This section describes sources of meteorology data and how it was processed through the PSU/NCAR Mesoscale Model version 5 (MM5) to produce the required meteorological fields. Both CALPUFF and CMAQ air quality model, described in Section 3, require meteorology data as inputs. After the meteorological fields were produced with MM5, the Meteorological Chemical Interface Processor (MCIP) was used to generate meteorological fields for CMAQ, and the CALMM5/CALMET preprocessors were used for CALPUFF. This section describes how MM5 was used to generate the meteorological fields. The post-processing of the MM5 outputs with MCIP and CALMET is described in Section 4.

1.1 Mesoscale Model Version 5 (MM5)

The meteorology modeling used the MM5 to produce annual meteorological fields for use in the air quality models. The MM5 is a limited-area, terrain-following (sigma-coordinate), prognostic meteorological model that solves the full suite of non-hydrostatic prognostic primitive equations for three-dimensional wind, temperature, water (in all phases), and pressure fields. It can be run with multiple one-way or two-way nested grids to resolve a range of atmospheric processes and circulations on spatial scales, ranging from one to several thousands of kilometers. The model is highly modular, facilitating the interchange of physics and data assimilation options. Several options exist for boundary layer schemes; resolved and sub-grid cloud and precipitation treatments; soil heat budget models; and radiative transfer. The model equations are solved horizontally on an Arakawa-B grid structure defined on a number of available map projections.

The Lambert conformal conic projection is used for air quality applications in the United States. The vertical coordinate is a terrain-following normalized pressure coordinate, referred to as a "sigma-p". Typically, 30–50 vertical levels are used to resolve the troposphere and lower stratosphere to ~15 km (~9 miles).

The model is supported by several pre- and post-processing programs, which are referred to collectively as the *MM5 modeling system.* The MM5 modeling system software is written mostly in Fortran, and has been developed at Penn State and NCAR as a community mesoscale model with contributions from users worldwide. The pre- and post-processing tools facilitate the development of various model inputs, and the analysis of model output.

Because MM5 is a limited-area model, it requires lateral boundary conditions that define the space- and time-varying conditions at the periphery of the coarsest domain throughout the simulation. Both initial and boundary conditions are generally specified using observational analyses, and may be supplemented by additional surface or upper air observations. These data sources can be obtained from a variety of routine analysis systems, from several global analysis products to higher resolution (time and space) forecast initialization fields prepared by the National Weather Service or other entities. Most datasets are available directly from NCAR.

The model may be constrained during the simulation to relax toward observed temperature, wind, and humidity observations through the use of four-dimensional data assimilation, known

as FDDA (Stauffer and Seaman 1990, 1991. FDDA amounts to adding an additional term to the prognostic equations that serves to "nudge" the model solution toward objective analysis fields and/or individual observations. This nudging has been shown to significantly reduce drift in the solution for simulations of several days or more. Drift may be caused by (among other effects) inaccuracies in the initial conditions, the effects of discretization, or errors in the formulation of various parameterizations.

1.2 MM5 Configuration

The MM5 modeling system configuration for the 2002 annual simulation for this project was built on the prior 2002 Western Regional Air Partnership (WRAP) MM5 application performed by UC Riverside and ENVIRON (WRAP 2002 MM5 Modeling Protocol, 2004), which was in turn set according to the optimal MM5 physics options that resulted from an in-depth sensitivity project carried out by Illinois Department of Natural Resources (IDNR) and the Lake Michigan Air Directors Consortium (LADCO). The MM5 simulations that were carried out for this project used the latest available version of the model (v3.6.2).

1.3 MM5 Domain

MM5 was configured to run two grids: (1) the continental-scale Regional Planning Organization (RPO) National Grid with 36-km grid point spacing, and an Nitrogen Deposition (NDEP) specific California grid with 4-km grid point spacing (Figure A-1). The model simulations were performed on these grids individually. This approach is usually referred to as "one-way" nesting. In this approach, MM5 is first run on the 36 km grid, and then boundary conditions are extracted from the resulting fields with the "Nestdown" preprocessor to provide initial and continuous boundary conditions for the 4 km simulation. Therefore, information passes one-way from the 36-km outer domain to the 4-km nested domain.

The MM5 uses a spherical earth. The RPO National Grid is defined on a Lambert conformal projection, with true latitudes at 33°N and 45°N, and the central latitude and longitude at 40°N and 97°W, respectively. The grid point spacing is 36 km. The continental expanse of this domain results in a grid of 165 (east-west) by 129 (north-south) dot points, and 164 (east-west) by 128 (north-south) cross points (Figure A-1). Overall, the 36-km domain covers 5904 km by 4608 km. The 4-km California domain is also defined on a Lambert conformal projection with identical true latitudes and center of the projection to the 36-km domain. There are 244 dot points (243 grid cells) in the north-south direction and 172 dot points (171 grid cells) in the east-west direction.

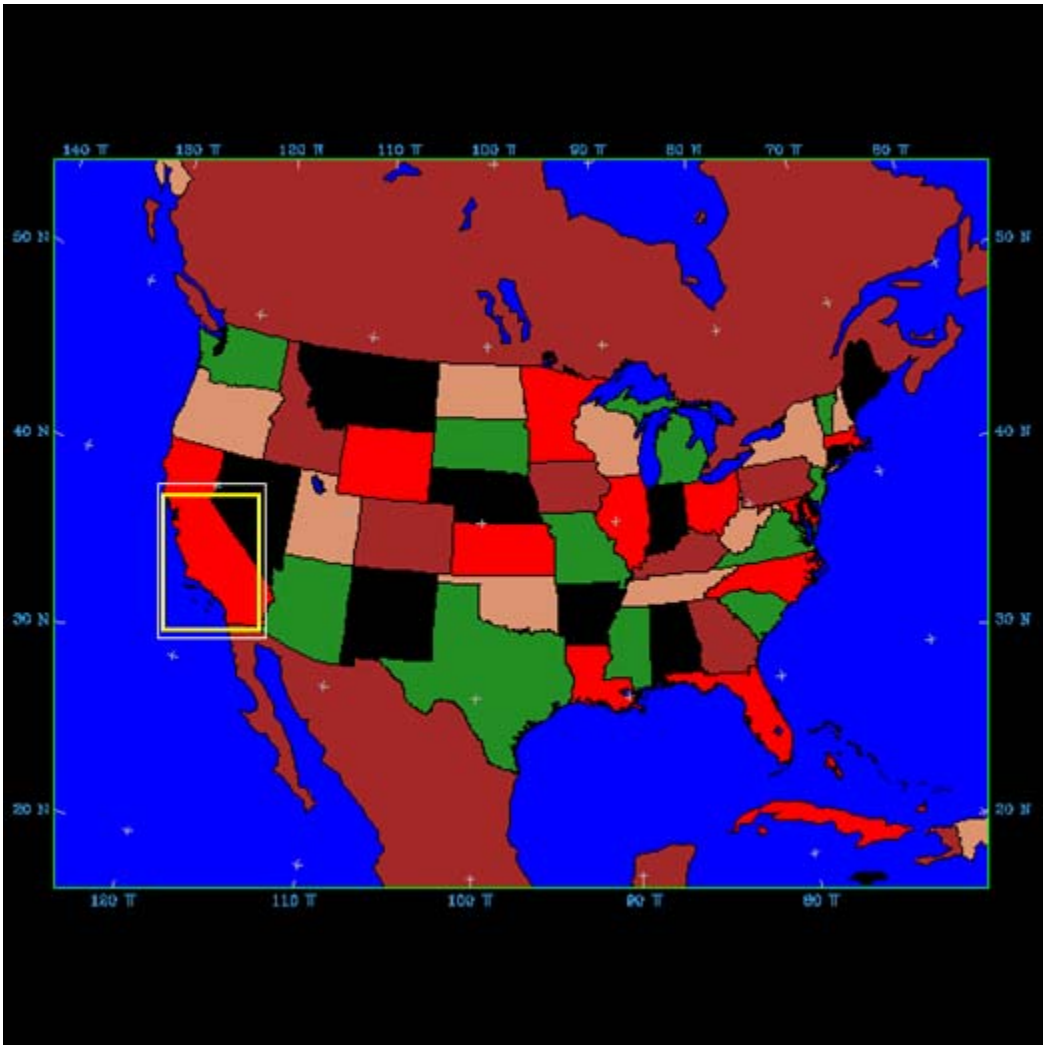


Figure A-1. MM5 modeling domains for 36-km (D01, national) and 4-km (D02, California) grid cells. The 4-km CMAQ domain nested within the 4-km MM5 domain is shown in yellow.

1.4 Vertical Grid Structure

The WRAP 2002 MM5 36-km simulations were performed with a 34 layer vertical structure. In order to reduce run-time for the 4-km MM5 simulations, we collapsed the 34 vertical layers into 19 vertical layers that match exactly with the 19 vertical layers in CMAQ domain. The collapsing of 34 into 19 layers occurred at the "nestdown" process. The layer structures are summarized in Table A-1. The altitudes above sea level are estimated according to standard atmosphere assumptions used in MM5 (surface pressure of 1000 millibar (mb), model top at 100 mb, surface temperature of 275° kelvin (K) (35°F), and log-pressure (ln[p]) lapse rate of 50 K/ln[p]).

Table A-1. MM5 vertical layer structure for the N-DEP 2002 application.

36-km Layers	Sigma	Pressure (mb)	Height (m)	4-km Layers
34 (model top)	0.000	100	14662	19 (model top)
33	0.050	145	12822	
32	0.100	190	11356	
31	0.150	235	10127	
30	0.200	280	9066	
39	0.250	325	8127	18
28	0.300	370	7284	
27	0.350	415	6517	
26	0.400	460	5812	
25	0.450	505	5160	17
24	0.500	550	4553	
23	0.550	595	3948	
22	0.600	640	3448	16
21	0.650	685	2942	
20	0.700	730	2462	15
19	0.740	766	2095	
18	0.770	793	1828	14
17	0.800	820	1569	
16	0.820	838	1400	13
15	0.840	856	1235	
14	0.860	874	1071	12
13	0.880	892	911	11
12	0.900	910	753	10
11	0.910	919	675	
10	0.920	928	598	9
9	0.930	937	521	
8	0.940	946	445	8
7	0.950	955	369	7
6	0.960	964	294	6
5	0.970	973	220	5
4	0.980	982	146	4
3	0.985	987	109	3
2	0.990	991	73	2
1	0.995	996	36	1
0 (ground)	1.000	1000	0	0 (ground)

m=meters

1.5 Physical Treatments and FDDA

The key physics options selected for the 2002 36-km and 4-km domains are shown in Table A-2. The Reisner II cloud microphysics scheme (Reisner et al. 1998) was selected because the EPA recommends that a mixed-phase ice scheme be employed in MM5 to drive aqueous chemistry and wet scavenging in CMAQ. Selection of the Pleim-Xiu land surface model (Xiu and Pleim 2000) required the use of the Asymmetric Convective PBL option (Pleim and Chang 1992), because these two are directly coupled. The Pleim-Xiu (P-X) parameterization is a predictive/interactive soil temperature and moisture budget model that responds to atmospheric processes that affect the thermodynamics of the surface (e.g., rainfall), while in turn dictating the surface fluxes of momentum, heat, and moisture into the boundary layer to further affect atmospheric processes. This allows the P-X approach to maintain a historical "memory" of the soil conditions over the course of a continuous simulation. It also allows the P-X deposition routines to be used in CMAQ.

Table A-2. Physics options selected for the 2002 WRAP MM5 simulation

Physics Option	Parameterization
Cloud Microphysics	Reisner II
Cumulus Parameterization	Kain-Fritsch
Planetary Boundary Layer	Asymmetric Convective Mixing Model
Land Surface Model	Pleim-Xiu (no INTERPPX)
Radiation	Rapid Radiative Transfer Model
Shallow Convection	None
Varying SST with time?	Yes
Thermal Roughness	Garratt
Snow Cover	Simple snow model

MM5 was configured to utilize its FDDA capabilities to nudge the model toward observed wind, temperature, and moisture fields throughout the 2002 annual simulation for the 36-km domain, but no FDDA was performed for the 4-km nested domain. Analysis (or grid) nudging was performed at 3-hour intervals both for the two-dimensional surface fields and for the three-dimensional fields aloft, excluding the boundary layer depth. Exclusion of the boundary layer in the FDDA process removes the potential of squelching out resolved mesoscale forcing in the model that are important to boundary layer development and thus the vertical fluxes of momentum, heat, and moisture into the free atmosphere and to the surface. Analysis nudging coefficients are shown in Table A-3. Use of FDDA to nudge toward observational data at individual measurement sites (i.e., "station" or "observation" nudging) was not performed. Usually, this option is best suited for smaller, high-resolution grids in which data from a very dense network of measurement sites are available (such as an intensive field study).

2 Procedure to Simulate the Year 2002 for 4-km Domain Preprocessing

Two key preprocessing steps are necessary to prepare input data for a 4-km MM5 simulation from the 36-km MM5 results. The MM5 modeling system provides all of the preprocessors necessary to prepare topographic, vegetative, initial condition, boundary condition, and FDDA nudging input files. The two preprocessors are summarized in Table A-4. Global topographic data at 10-minute (latitude/longitude) resolution was used to define terrain elevations on the 36-km grid; higher two-minute resolution from the same dataset will be used for the smaller 4-km domain.

Land use distribution on the MM5 domains were defined from the 24-category United States Geological Survey (USGS) vegetation data, with a resolution of 10 minutes. The TERRAIN processor was run with options invoked to process all of the additional terrestrial information necessary to run the P-X land surface model. Figure A-2 shows the terrain height and the dominant vegetation and land use type.

Table A-3. Four Dimensional Data Assimilation (FDDA) analysis nudging coefficients (second^{-1}).

Wind	2.5×10^{-4}
Temperature	2.5×10^{-4}
Water vapor	1×10^{-5}

Table A-4. Description of MM5 Pre-Preprocessors.

Program	Description
TERRAIN	Defines the MM5 horizontal domain specifications, including nested grid relationships; processes raw topographic, vegetative, and soil type data to all MM5 grids.
NESTDOWN	The NESTDOWN program horizontally interpolates σ–coordinate data, from a coarse grid to a fine grid. Collapsing of layers from 34 to 19 vertical levels occur in this preprocessor. The advantages to use this program to produce a higher resolution model run from a coarse grid are: (1) the model has lateral boundary conditions that use consistent physics with the coarse grid model; (2) the lateral boundary conditions are available at a relatively high temporal frequency; and (3) the vertical structure of the atmosphere is not significantly modified through vertical interpolation. Without the inclusion of observations, though, the model may drift.

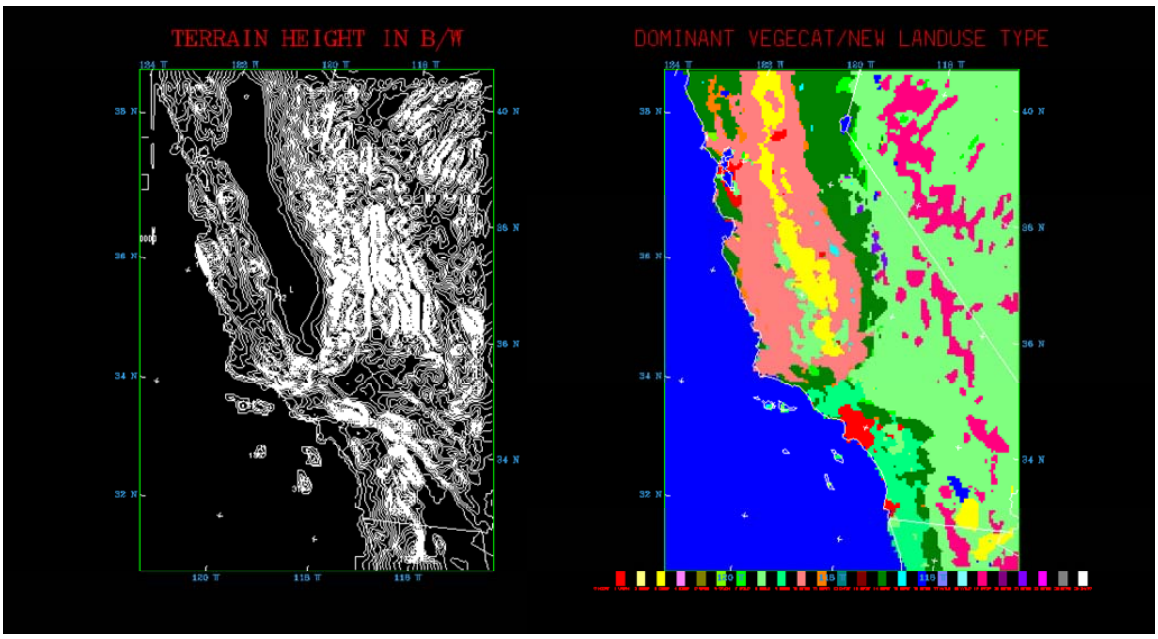


Figure A-2. MM5 4-km domain terrain height, shown in black and white (left plot); and the dominant vegetation and land use type (right plot)

2.1 Model Application

The annual simulation was made in sequential five-day run segments, each with an initial spinup period of 12 hours that overlapped the last 12 hours of the preceding run. This overlapping is included so that the air quality model can be started at either 0Z or 12Z without including the MM5 re-initialization period. MM5 will be re-initialized at the beginning of each 5-day period to reduce error propagation through the simulation. The 2002 annual simulation includes the final two weeks of December 2001 to allow for sufficient spin-up time for photochemical/visibility applications with start dates at the beginning of January 2002. A list of the run segments and their date/time durations are provided at http://pah.cert.ucr.edu/aqm/308/mm5.shtml. The model was run with 90- and 10-second time steps on the 36-km and 4-km grids, respectively.

3 Evaluation of the 2002 Annual Run

The goal of the evaluation was to determine whether the meteorological fields were sufficiently accurate to properly characterize the transport, chemistry, and removal processes in CMAQ. If errors in the meteorological fields are too large, the ability of the air quality model to replicate regional pollutant levels over the entire base year will be severely hampered and the predicted impacts from future year growth and controls will be highly questionable.

Previous peer-reviewed documentation of MM5 formulation, testing, and evaluation provide the basis for the scientific evaluation. The "Interim Report: 2002 Annual MM5 36 km Simulation to Support WRAP CMAQ Visibility Modeling for the Section 308 SIP/TIP" (http://pah.cert.ucr.edu/aqm/308/mm5_reports04.shtml) provides a preliminary analysis on the MM5 model performance for the 2002 36km annual simulation. This evaluation was limited to: (1) the comparison of the 4-km nested domain with the 36-km domain for January and July, 2002; and (2) whether the predicted meteorological fields were reasonable and consistent, and agree adequately with available observations in time and space. The process provides only limited information about whether the results are correct from a scientific perspective or whether they are the fortuitous product of compensating errors; thus a "successful" operational evaluation is a necessary but insufficient condition for achieving a sound, reliable performance testing exercise.

Figures A-3 show MM5 January 4-km domain model performance bias for surface temperature and wind velocity. Figures A-4 and A-5 show the model performance between observed and model predicted temperature and humidity fields. In January, the model tends to under-predict the maximum temperature for each day and over-estimate the minimum temperature. For humidity, the model does a fairly reasonable good job of reproducing observation results.

Figure A-6 show the temperature and wind speed bias for the July MM5 runs. The model shows a tendency to under-predict both temperature and wind speed. Figure A-7 shows observed versus model predicted temperature for July. The MM5 runs slightly under-estimates the peak temperature in the afternoon but does a fairly good job reproducing the daily minimum temperature. No phase lag in model predicted temperature was observed. The July observed versus predicted humidity plot (Figure A-8) shows under-prediction in most days.

Comparisons between the WRAP 36-km MM5 runs and the Nitrogen Deposition 4-km for the California domain show that the 4-km domain produced a higher bias for wind speed (Figure A-9), wind direction (Figure A-10), and temperature (Figure A-11). However, we determined that the difference is not large enough to cause major concerns with the MM5 simulation results.

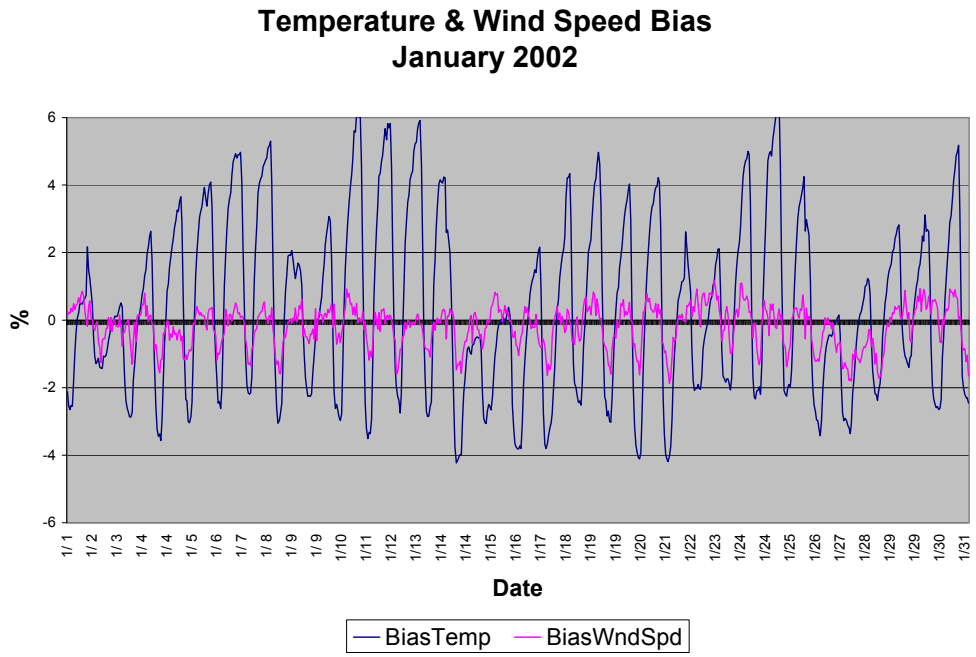


Figure A-3. January 2002 N-DEP 4-km domain MM5 model performance bias for surface temperature and wind speed

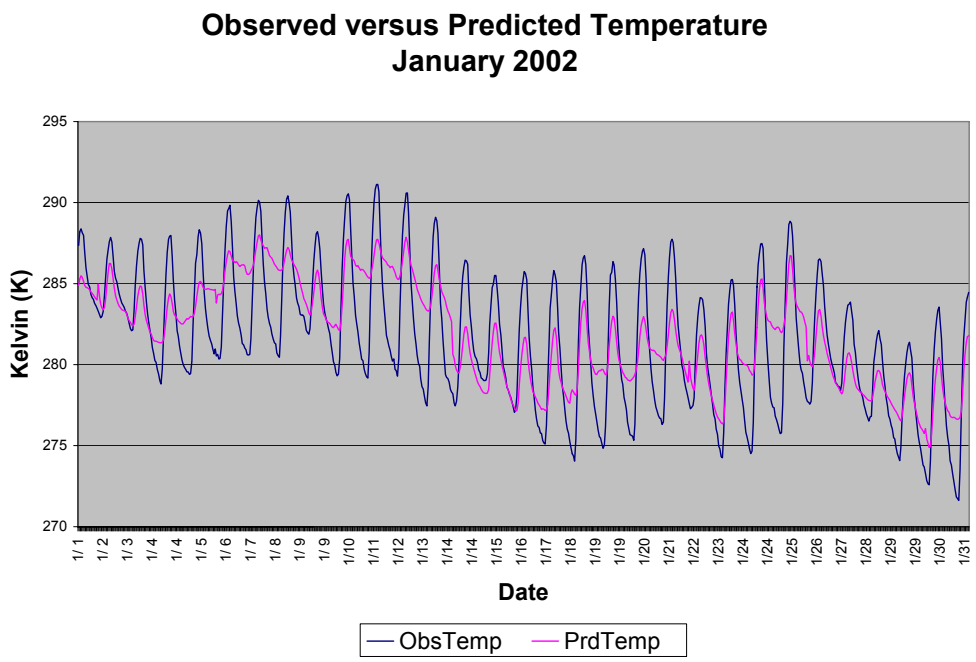


Figure A-4. January 2002 N-DEP 4-km domain MM5 model performance between observed and model predicted temperature fields

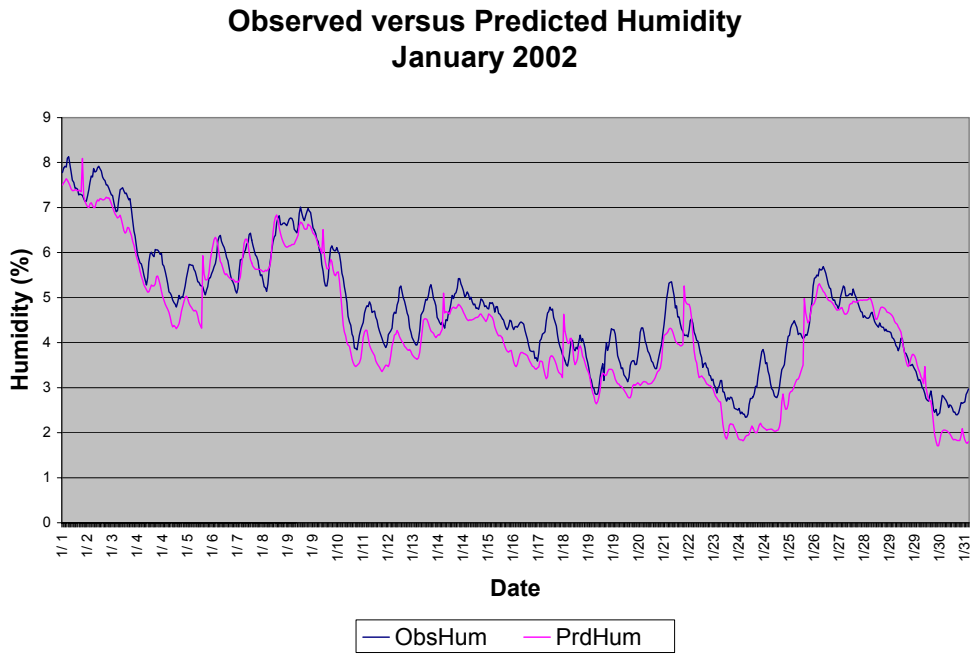


Figure A-5. January 2002 N-DEP 4-km domain MM5 model performance between observed and model predicted humidity fields

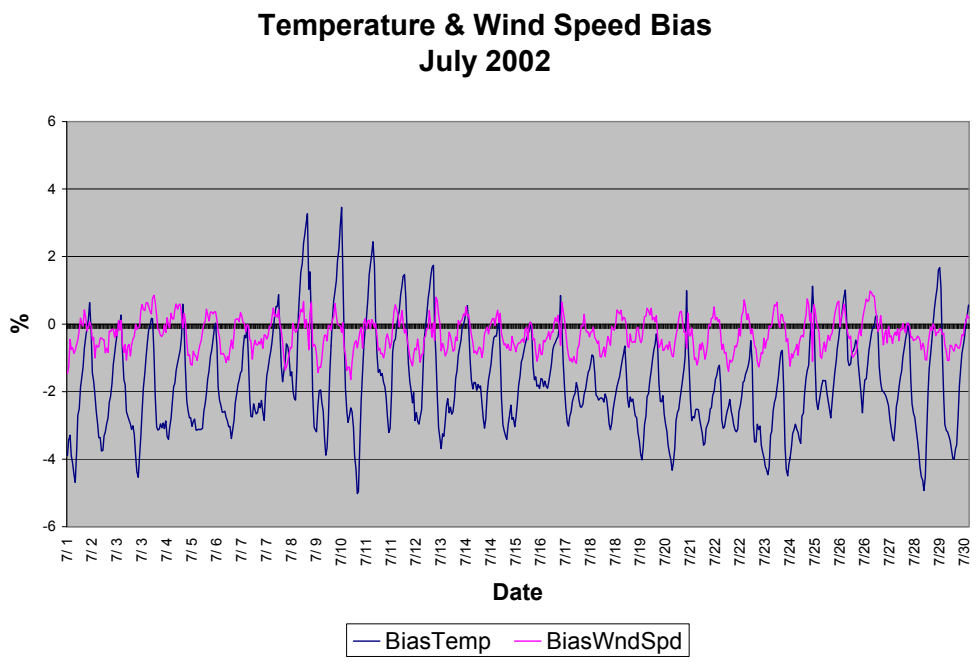


Figure A-6.July 2002 N-DEP 4-km domain MM5 model performance bias for surface temperature and wind speed

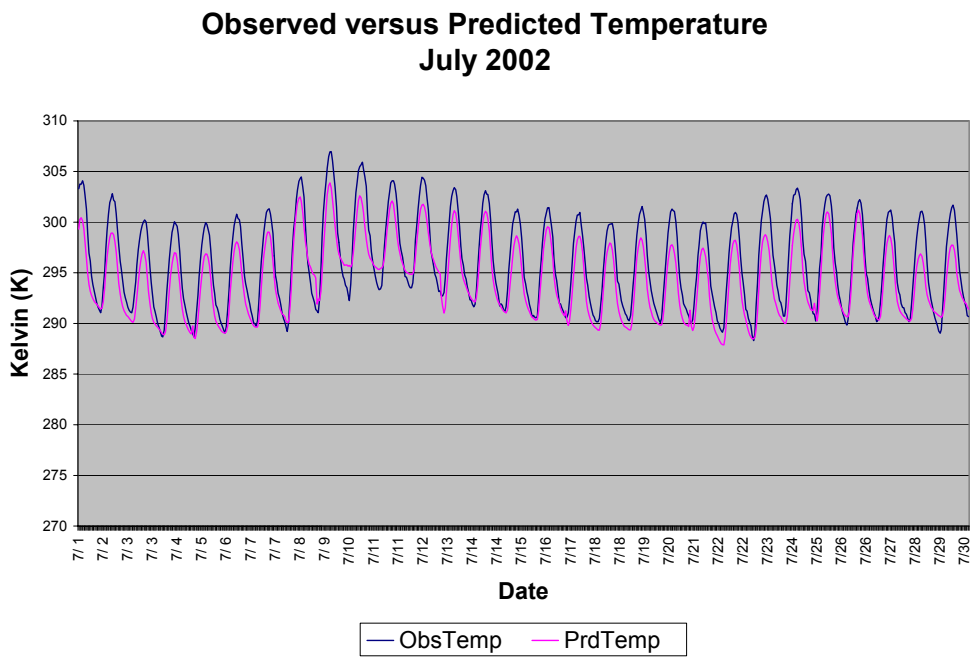


Figure A-7. July 2002 N-DEP 4-km domain MM5 model performance between observed and model predicted temperature fields

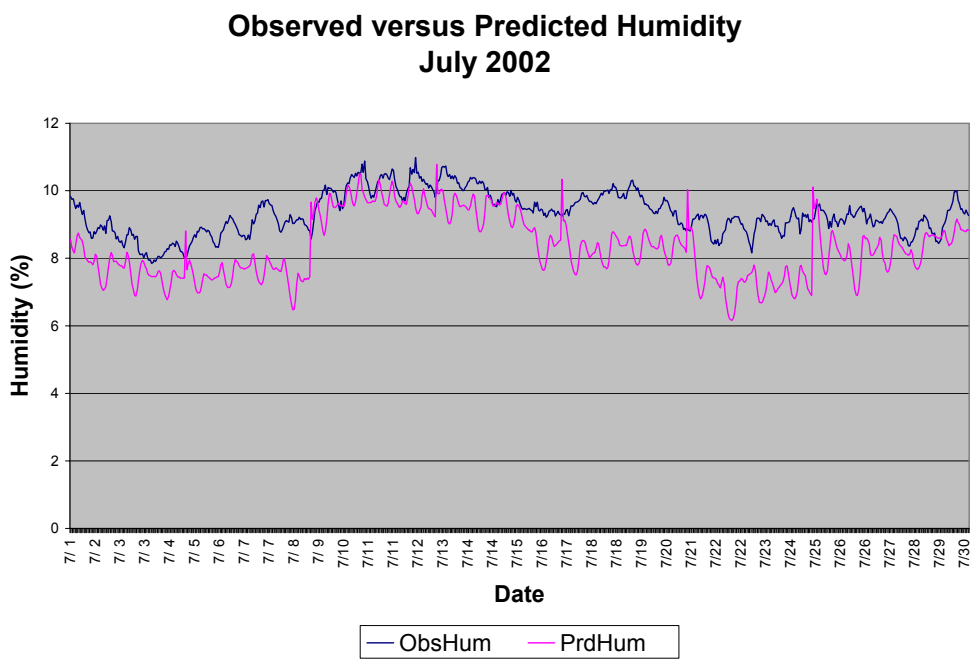


Figure A-8. July 2002 N-DEP 4-km domain MM5 model performance between observed and model predicted humidity fields

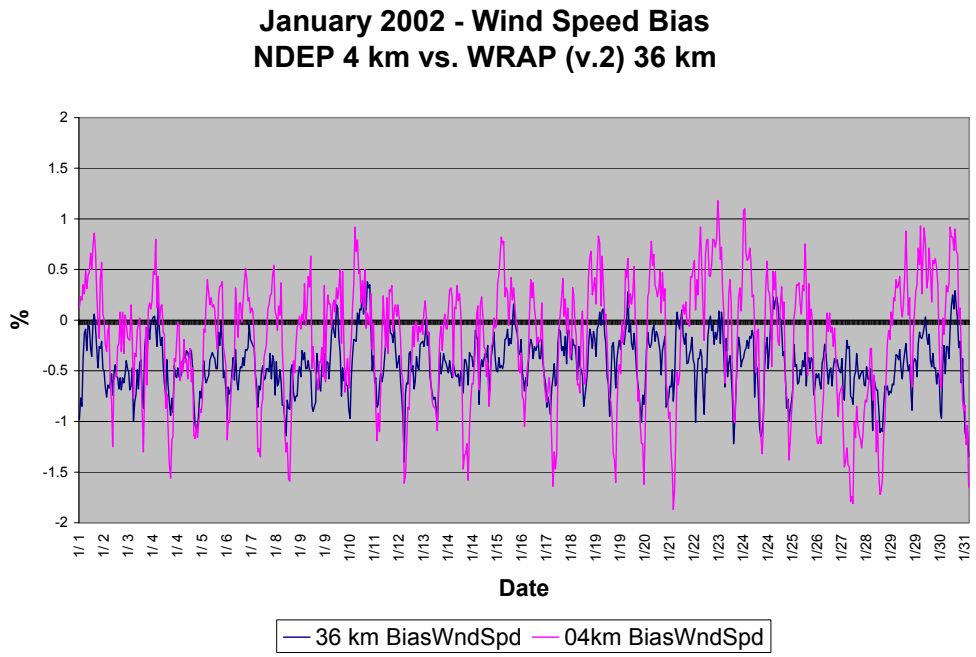


Figure A-9. January 2002 MM5 surface wind velocity bias comparison between the N-DEP 4-km domain and the WRAP 36-km MM5 results, for those sites that are located in the N-DEP 4-km region

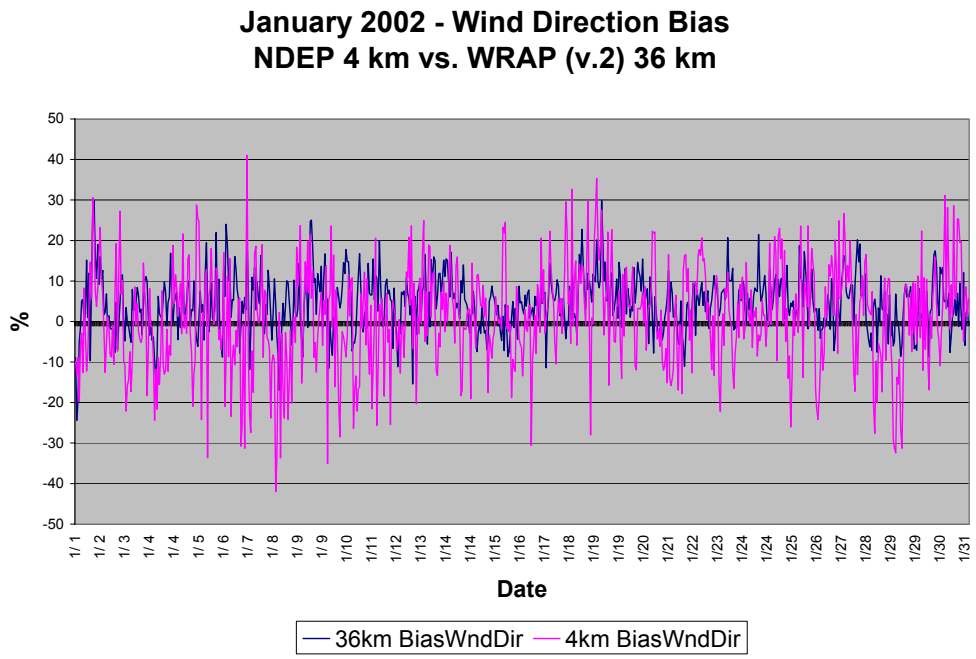


Figure A-10. January 2002 MM5 surface wind direction bias comparison between N-DEP 4-km domain and WRAP 36 km MM5 results that are in the N-DEP 4-km region

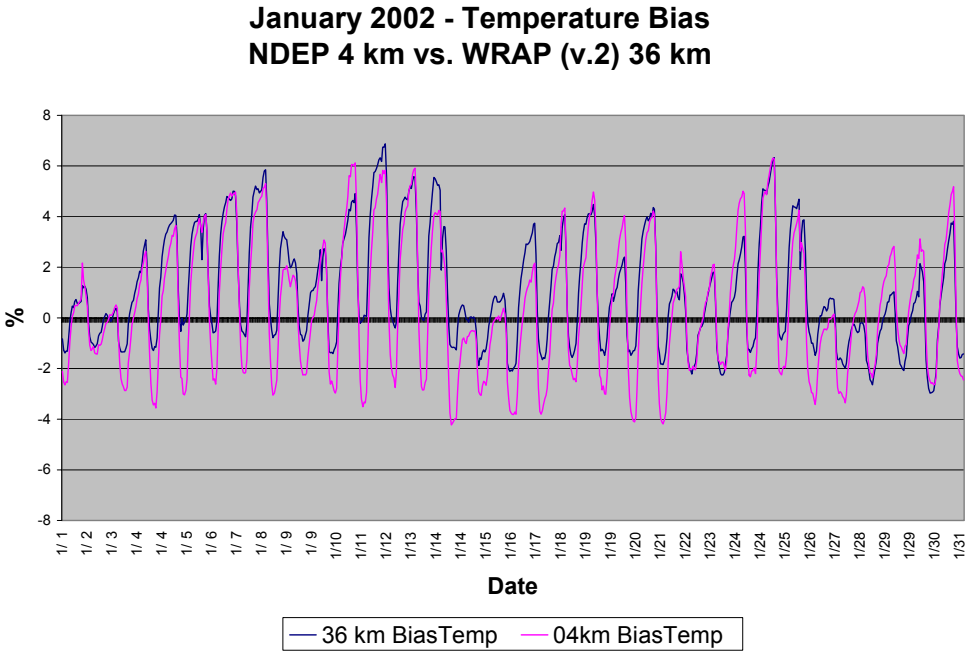


Figure A-11. January 2002 MM5 surface temperature bias comparison between N-DEP 4-km domain and WRAP 36-km MM5 results in the N-DEP 4-km region

Appendix B

Development of Emissions Inventory Data for the 4-km CMAQ Model

1 Emissions Input Data

Emissions input data for the Energy Commission 4-km domain have been extracted from WRAP 2002 emissions datasets. The emissions for the following source categories were processed for the month of July 2002:

1. Area source emissions
2. Point source emissions
3. Mobile emissions
4. Non road mobile emissions
5. Road dust
6. Off shore sources
7. Mexico emissions inventory
8. Biogenic gridded land use

The advantage of using the WRAP emission databases is that WRAP and other Regional Planning Organizations (RPOs) have devoted substantial resource to developing improved emissions inventories specifically for the RPO unified projection. Because errors and uncertainty in emissions inventories are the most important sources of uncertainty in air quality modeling studies, this N deposition study will benefit from these efforts by using the RPO grid.

2 Emissions Processing

2.1 SMOKE Background

The purpose of SMOKE (or any emissions processor) is to convert the resolution of the emission inventory data to the resolution needed by an air quality model. Emission inventories are typically available with an annual total emissions value per county for each emissions source, or perhaps with an average-day emissions value. The air quality models, however, typically require emissions data on an hourly basis, for each model grid cell (and perhaps model layer), and for each model species. Consequently, emissions processing involves (at a minimum) transformation of emission inventory data by temporal allocation, chemical speciation, spatial allocation, and perhaps layer assignment, to achieve the input requirements of the air quality model. The biogenic emissions were processed with the Biogenic Emission Inventory System (BEIS), version 3.12, or BEIS3.12.

SMOKE formulates emissions modeling in terms of sparse matrix operations. Figure B-1 shows an example of how the matrix approach organizes the emissions-processing steps for anthropogenic emissions, with the final step in creating the model-ready emissions being the merge step. This example does not include all processing steps (which can be different for each source category in SMOKE) but does include the major processing steps listed in the previous paragraph, except the layer assignment. Specifically, the inventory emissions are arranged as a vector of emissions, with associated vectors that include characteristics about the sources such as its state and county (SCC). SMOKE also creates matrices that will apply the gridding, speciation, and temporal factors to the vector of emissions. In many cases, these matrices are

independent from one another, and can therefore be generated in parallel. The processing approach ends with the merge step, which combines the inventory emissions vector with the control, speciation, gridding and temporal matrices to create model-ready emissions. In case of sources with elevated emissions, such as fires and point sources, a matrix with emission fractions in each vertical layer is created and merged with other matrices.

For the temporal processing step, one can elect to process using representative Mondays, weekdays, Saturdays, and Sundays for each month; herein referred to as *MWSS processing.* This approach significantly reduces the number of times the temporal processing step must be run. The sections below identify the cases in which we used this processing approach.

In addition, Figure B-2 provides a schematic diagram of SMOKE/BEIS3.12 processing steps used in this project and shows the input and output files for the Normbeis3 program. The input files are the emission factors file (B3FAC), the gridded land use file for the first 120 land use types (BELD3_A and BELD3_B), and the land use totals data file (BELD3_TOT).

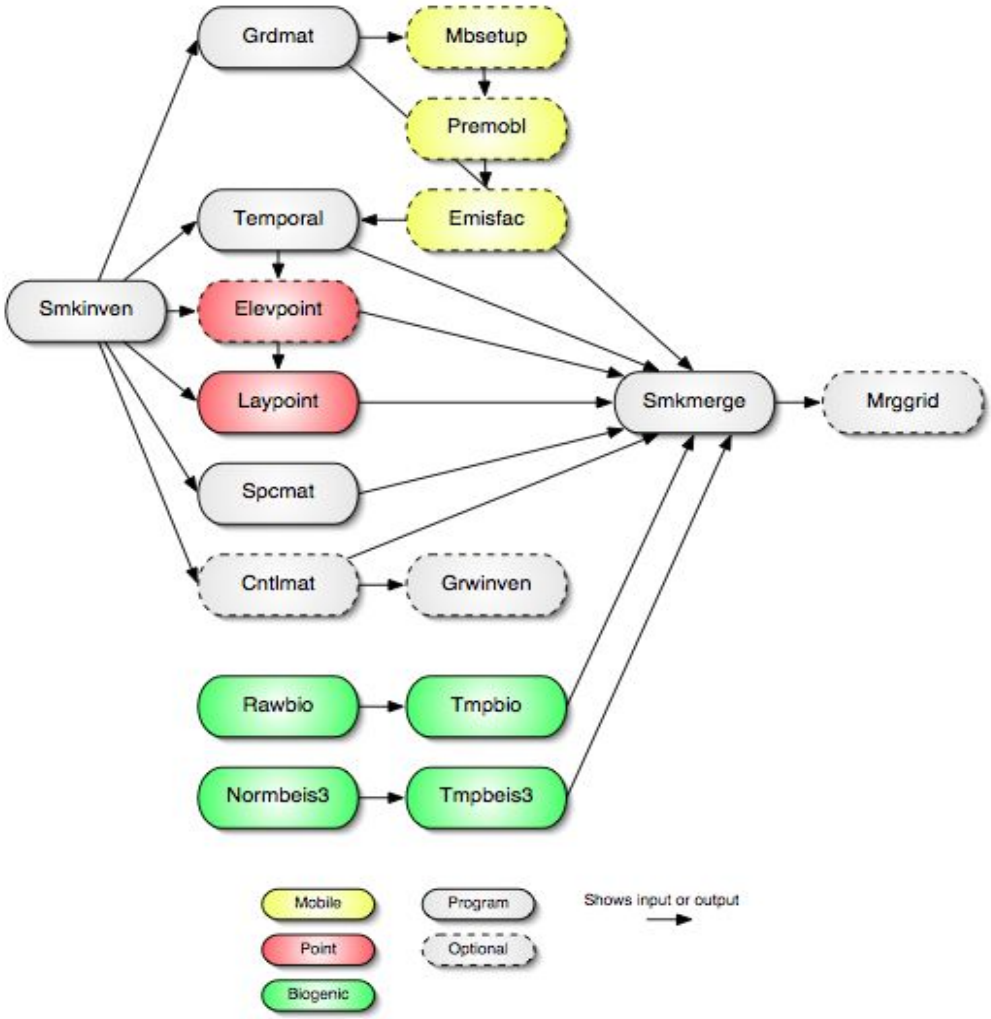


Figure B-1. Flow diagram of major SMOKE processing steps needed by all source categories. (Figure is reproduced from the SMOKE users manual, CEP, 2004.)

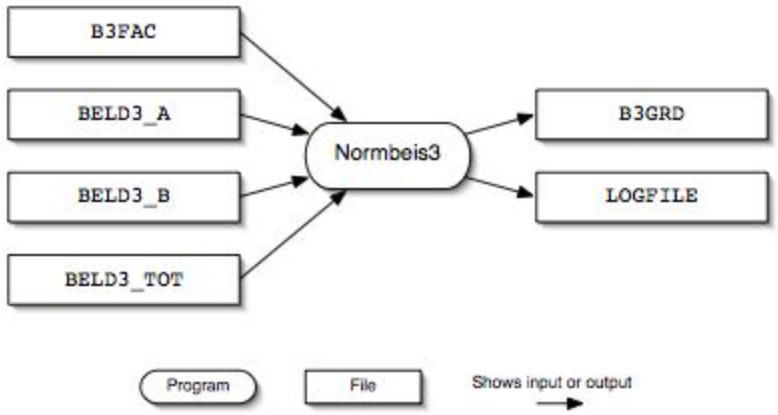


Figure B-2. Flow diagram of SMOKE/BEIS3.12 processing steps. (Figure is reproduced from the SMOKE users manual, CEP, 2004).

2.2 SMOKE Scripts

The scripts are the interface that emissions modelers use to run SMOKE, and are therefore the items of practical importance for anyone wanting to simply reproduce the work performed as part of this contract. For this project, we created many SMOKE scripts to run the required emissions modeling cases, which are described in this subsection. We did make several modifications to the default SMOKE scripts to modularize them, added error-checking loops, and broke up the reports and logs directories by source category. This resulted in one script for each source category being modeled that calls all of the SMOKE programs required for simulating that source.

2.3 Emission Inventory Quality Assurance

Quality assurance (QA) of the emissions inventory followed a QA protocol that was developed by the University of North Carolina, Carolina Environmental Programs (UNC-CEP) and has been used successfully for other RPO inventory development projects (e.g., WRAP and the Visibility Improvement State and Tribal Association of the Southeast (VISTAS). The different types of analysis used in the QA process are listed in the Quality Assurance Project Plan (QAPP). The main features of the procedures were detailed in the QAPP and are summarized below.

2.4 QA of SMOKE Inputs and Processing

<u>Input Screening Error Checking Algorithms:</u> Although the SMOKE emissions model is used for emissions processing, some additional input error checking algorithms are used to screen the data and identify potential emission input errors. In addition, EPA has issued a revised stack QA and augmentation procedures memorandum that is used to identify and augment any outlying stacks.

SMOKE error messages: SMOKE provides various cautionary or warning messages during the emissions processing. These log files are reviewed for serious error messages. An archive of the log files is also maintained so that the error messages can be reviewed at a later date if necessary.

SMOKE emissions summaries: Built-in QA functions of the SMOKE processing system provide summaries of processed emissions as daily totals according to species, source category, and county and state boundaries. These summaries are compared with summary data prepared for the pre-processed emissions (e.g., state and county totals for emissions from the augmented emissions data). In addition, comparisons of state-level emission totals by source category before and after gridding are compared to ensure that no problems were encountered in the spatial allocation of emissions to modeling grid cells.

QA of Model-Ready Emissions

Post-processing programs which QA the final outputs from SMOKE were developed by the University of California, Riverside (UCR) as part of the WRAP project. The program was run for each inventory source (area, point, etc.) individually and for the merged inventory.

The purposes of the post processing QA are to:

- ensure that no region or state was dropped from the emissions inventory files;
- Ensure that the daily changes (week-days, week-ends, and holily days) are processed correctly, and that the seasonal changes are correct;
- Ensure that diurnal profiles of week-days and week-ends are used; and
- Ensure that the point sources were distributed properly into the vertical layers.

If any unexpected or unusual behavior of the processed inventory was discovered, then a more detailed quantitative QA was conducted using SMOKE reports. The QA/quality control (QC) post-processing program that reads the CMAQ-ready, input-output (I/O) application programming interface (API) emissions file formats for each of the major source categories (i.e., mobile, area, point, biogenic, fire) is used to produce the following plots:

- **Spatial Summary:** Emissions for all layers and for all 24 hours are summed and used to prepare PAVE plots showing the daily total emissions spatial distribution. The objective of this step is to identify errors in spatial distribution of emissions (Figure B-3). **Vertical Profile:** For point sources, the total emissions for each layer are summed and plotted to show the vertical distribution of emissions. These plots show the emissions on the x-axis for each model layer on the y-axis. The objective of this step is to identify possible errors in vertical distribution of emissions (Figure B-4).
- **Short (diurnal) Term Temporal Summary:** The domain-wide emissions totals for each hour are accumulated and time series plots prepared that display the diurnal variation in total hourly emissions. The objective of this step is to identify errors in temporal profiles (Figure B-5). Note that the reference time is GMT.
- Long-**Term Temporal Summary:** The domain-wide emissions totals for each day are accumulated and displayed as time series plots that show the daily total emissions across

the domain as a function of time. The objective of this step is to identify particular days for which emissions appear to be inconsistent with other days for no reason (e.g., not a weekend) and compare them against the general trend (Figure B-6).

The plots have been posted and can be viewed on the WRAP Regional Modeling Center (RMC) web-site: www.cert.ucr.edu/aqm/ndep/qa_cec2002.shtml.

Figures B-7 and Figure B-8 are chart pies showing the percentage contribution of each source to the total NO_x and SO_X in the entire domain for January. Figure B-9 show daily area source emission for NO, NO_2, NH_3, and ISOP in tons per day for July 2, 2002. Daily point source emissions total on the same day for the same four species are shown in Figure B-10. Daily total on-road mobile source emissions on July 2, 2002 for the same four species are shown in Figure B-11. The July 2002 monthly point source emissions total per day for NO, NH_3, and ISOP are shown in Figure B-12.

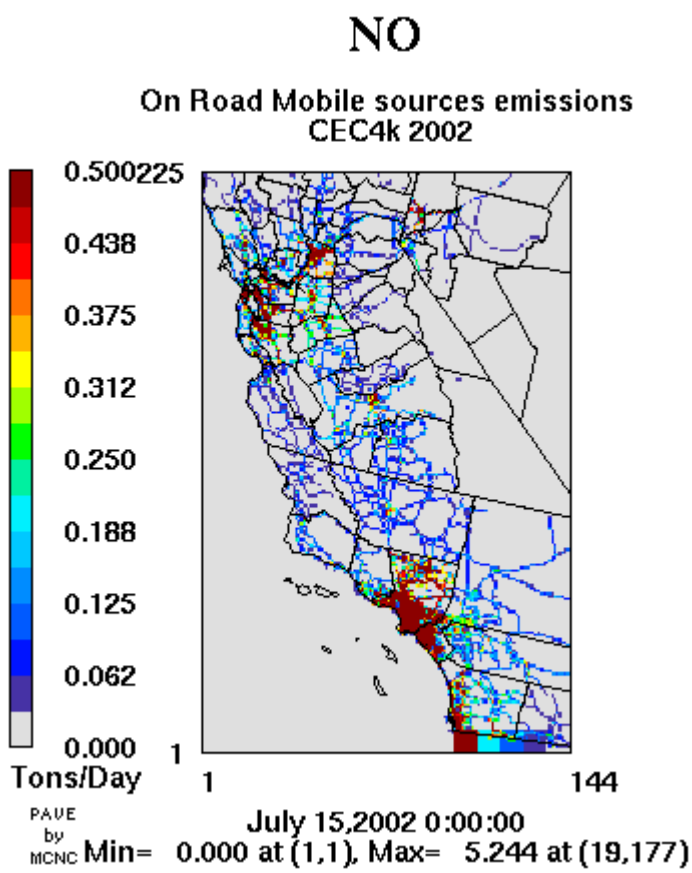


Figure B-3. On-road motor vehicle NO emissions for the Energy Commission 4-km domain for July 15, 2002

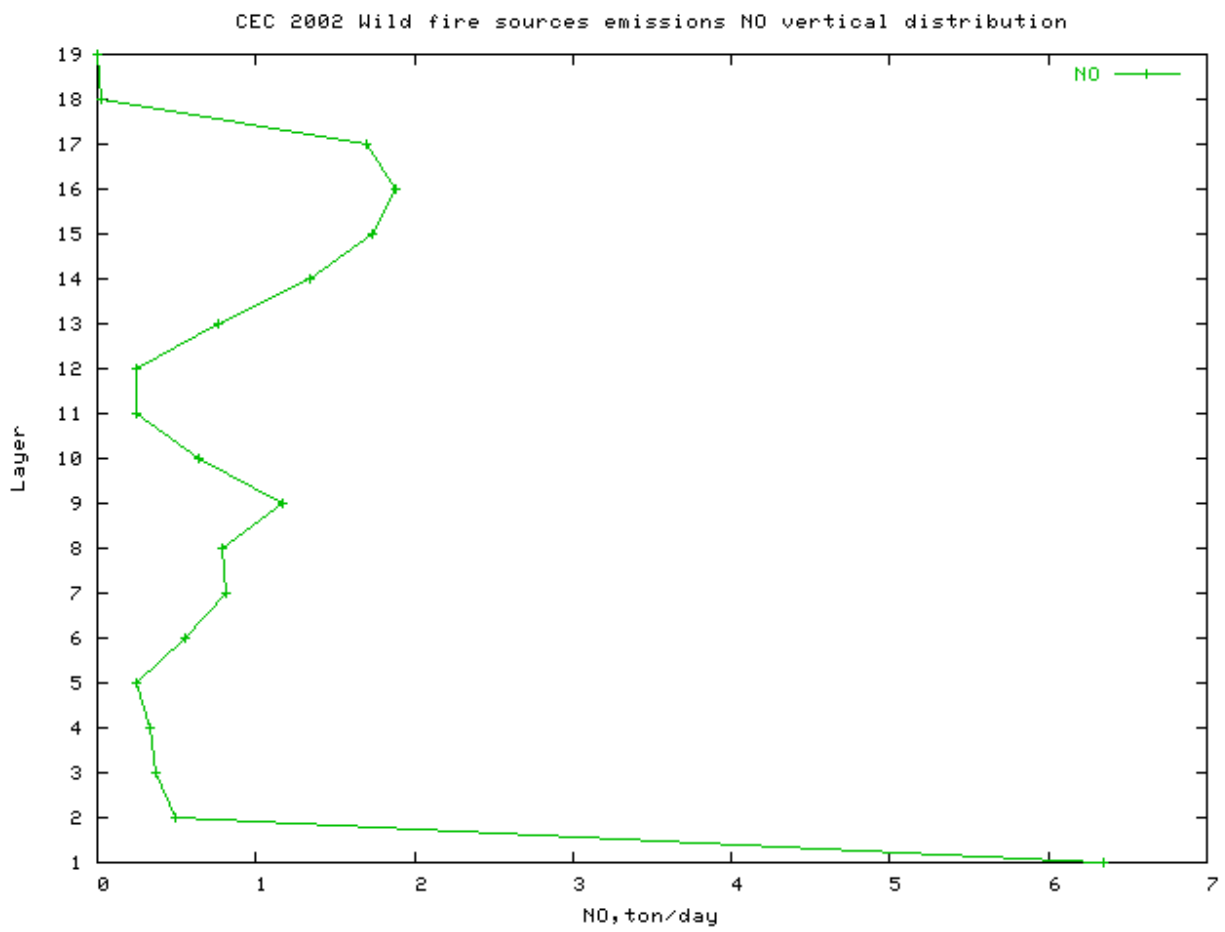


Figure B-4. Vertical profile for wildfire NO emissions

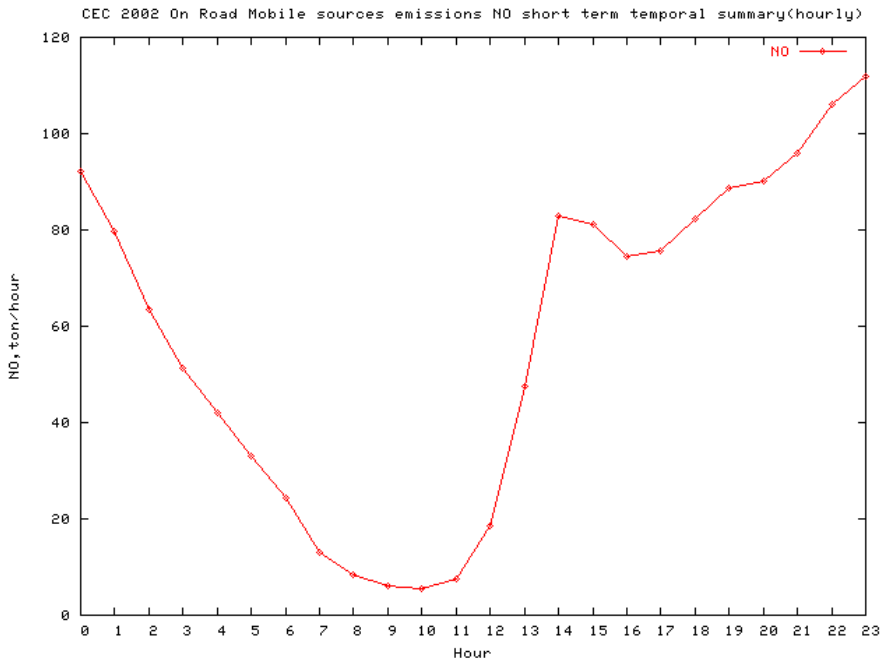


Figure B-5. On-road motor vehicle NO emissions for a 24 hour diurnal cycle (using GMT) for July 14-15, 2002

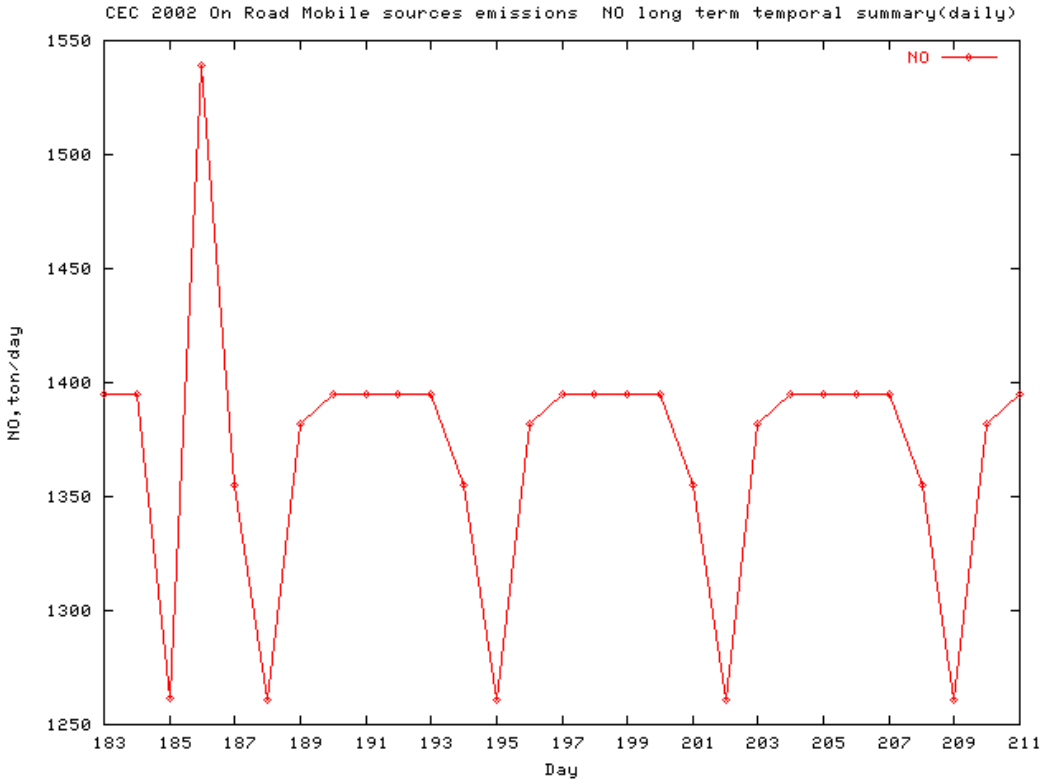


Figure B-6. On-road motor vehicle emissions from July 2 (183) to July 30 (211), 2002

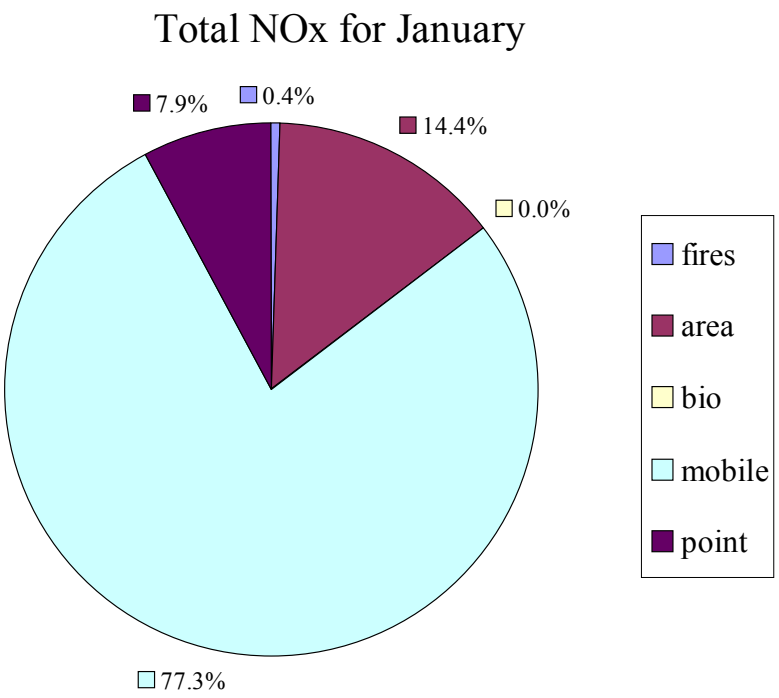


Figure B-7. Percentage of contribution from each source to the total NO_X during January

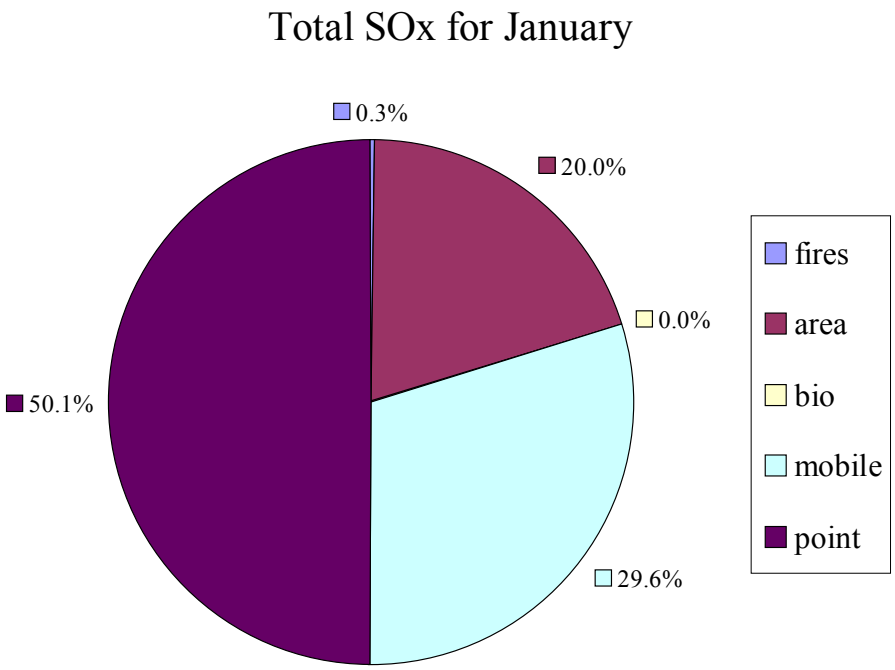


Figure B-8. Percentage of contribution from each source to the total SO_X during January

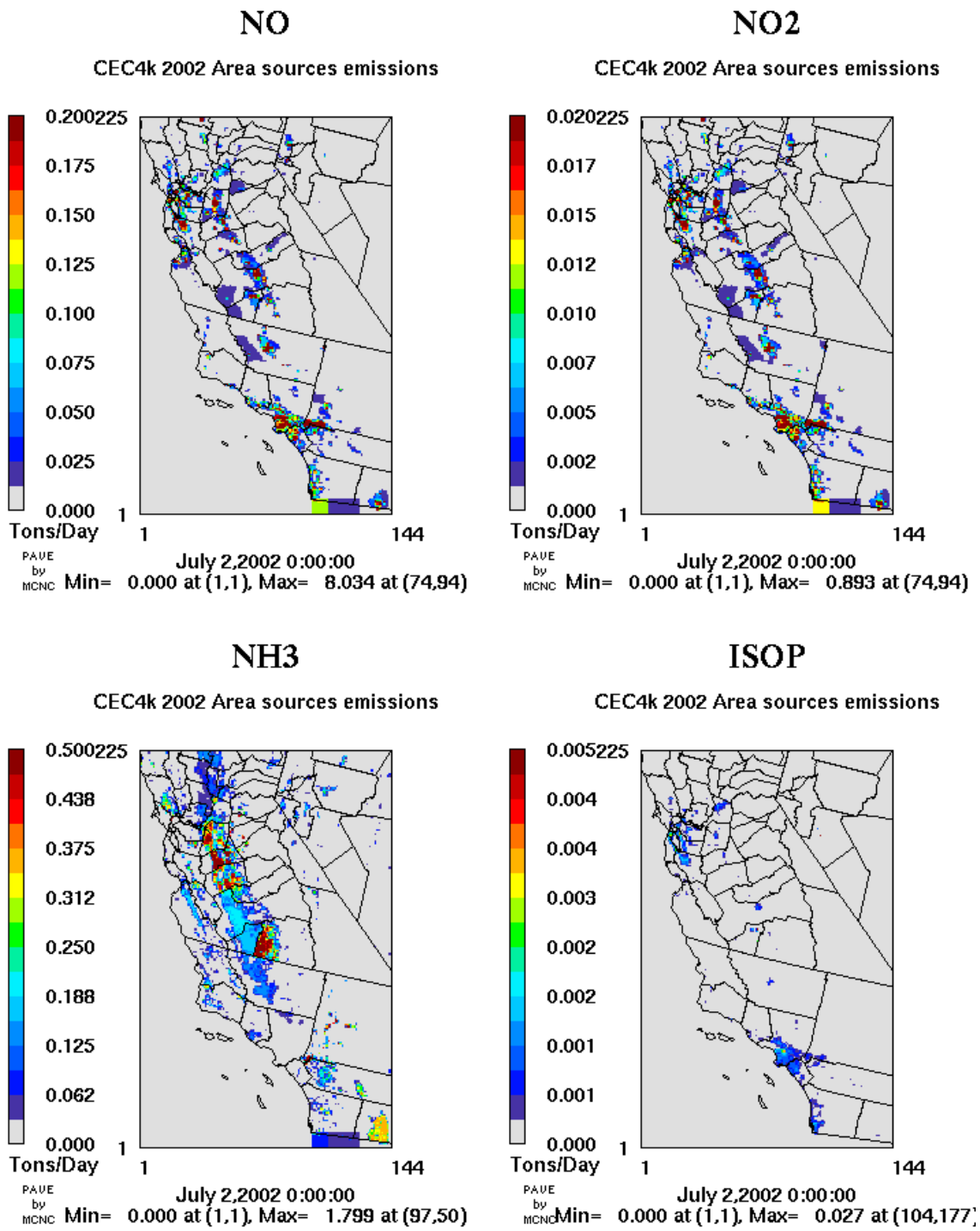


Figure B-9. July 2, 2002 daily total area source emissions for NO, NO_2, NH_3, and ISOP (isoprene) in tons/day

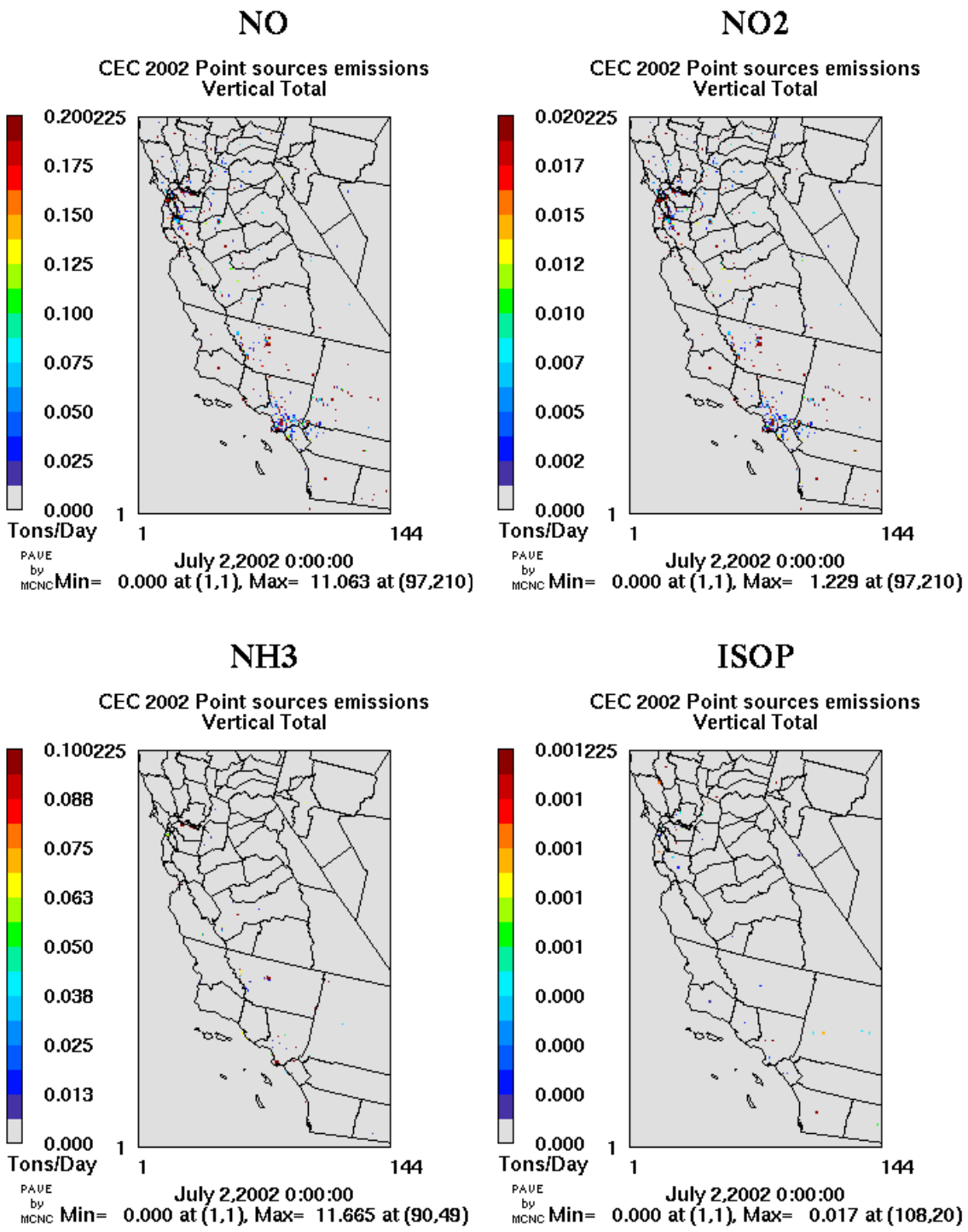


Figure B-10. July 2, 2002 daily total point source emissions for NO, NO_2, NH_3, and ISOP (isoprene) in tons/day

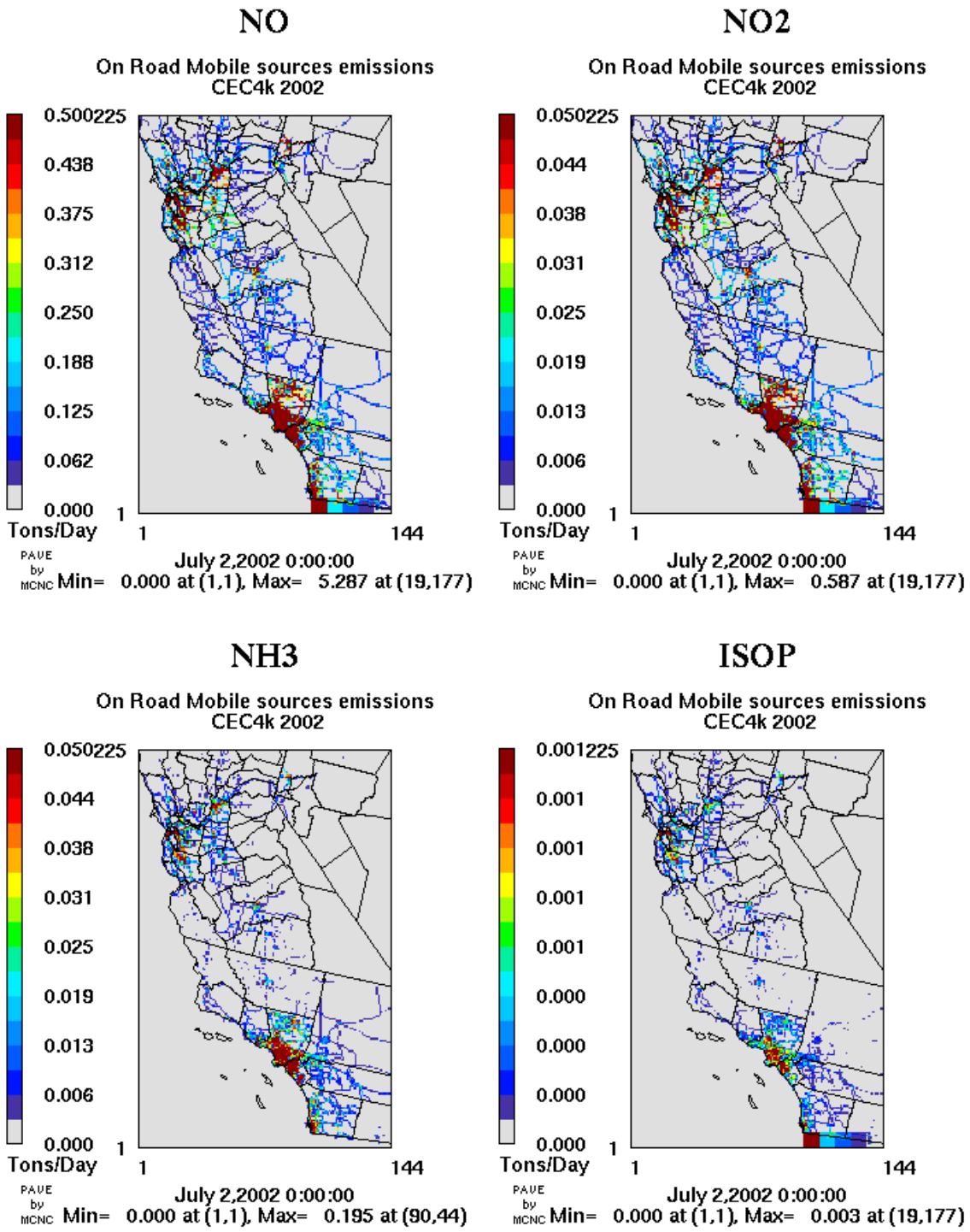


Figure B-11. July 2, 2002 daily total on-road mobile source emissions for NO, NO_2, NH_3, and ISOP (isoprene) in tons/day

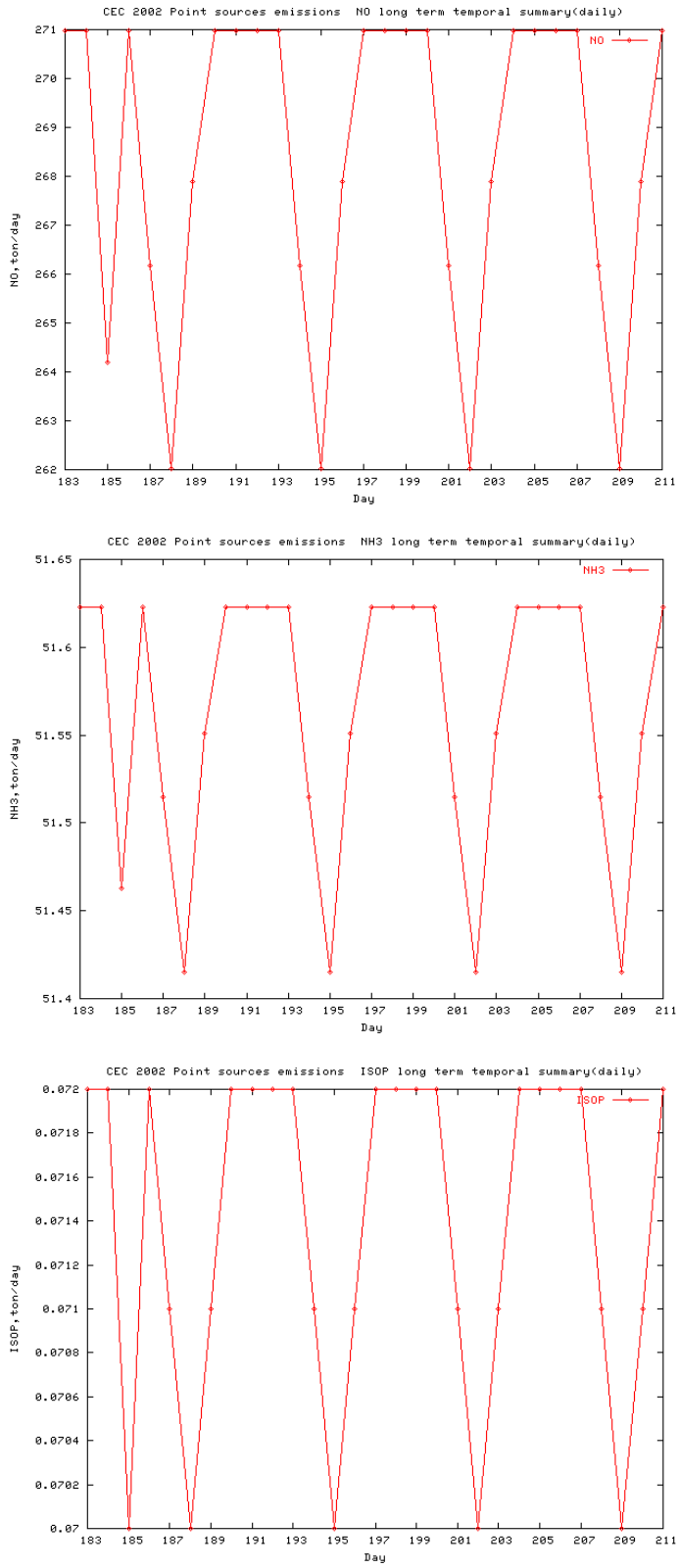


Figure B-12. July 2002 monthly point source emissions for NO, NH_3, and ISOP (isoprene) in tons/day

Appendix C

Description of Modeling Study Design and Model Configuration

1.0. CMAQ and CALPUFF Model Configurations

The N-DEP CMAQ and CALPUFF model configurations and sources of model-ready input files are described in this section. Default values and/or options are selected as the starting point. Subsequent sub-sections describe all specific modifications that were made to these inputs and model configurations for the various photochemical model sensitivity tests.

1.1 Modeling Domain

1.1.1 Horizontal Domain

In this study both the CALPUFF and CMAQ models use an identical domain, with 4-km resolution grid with 144 grid cells in the east-west direction and 225 grid cells in the north-south direction. The modeling domain is defined on a Lambert Conic Conformal mapping projection following the perfect sphere definition used in MM5. Four parameters essential for defining the Lambert projection for the N-DEP domain are as follows:

- True latitudes: 33°N and 45°N
- Central longitude: 97°W
- Projection origin: 97°W, 40°N

1.1.2 Vertical Grid Structure

The domain depth and the number of layers in the vertical for CALPUFF and CMAQ differ. The vertical layer structure for CMAQ simulations are based upon the MM5 mode. A total of 19 vertical layers extending from the ground to about 15,000 meters (13 miles) above sea level are used. No vertical layer collapsing was performed in processing the meteorological fields for CMAQ. For CALPUFF simulations, the vertical depth extends from the ground to 3000 meters (2 miles) above ground level (AGL). A total of 10 vertical levels are used in the CALPUFF simulations. The lowest level in MM5 was also divided into two vertical layers in CALPUFF. Table C-1 tabulates the vertical layer structure for both models.

1.1.3 CMAQ

The Community Multiscale Air Quality (CMAQ) modeling system is a "one-atmosphere" air quality modeling system developed by the EPA to address O_3, PM, air toxics, visibility, and acid deposition within a common platform (Dennis et al. 1996). The CMAQ is a system composed of a suite of models that preprocess the input data including meteorological fields, emissions inventories, initial condition, boundary conditions, and photolysis rates. The preprocessor provide the input for the CMAQ Chemical Tracer Model (CCTM), which is used to simulate the transport and chemical transformation, and fate of the emitted species (Tonnesen et al. 2003a).

This section describes the procedure for setting up and producing the necessary input files for CMAQ. Contrary to CALPUFF simulations, where Pacific Standard Time (PST) was used, all CMAQ simulation were performed in Coordinated Universal Time (UTC)—sometimes referred to as Greenwich Mean Time (GMT). The CMAQ-ready input files were all produced in UTC.

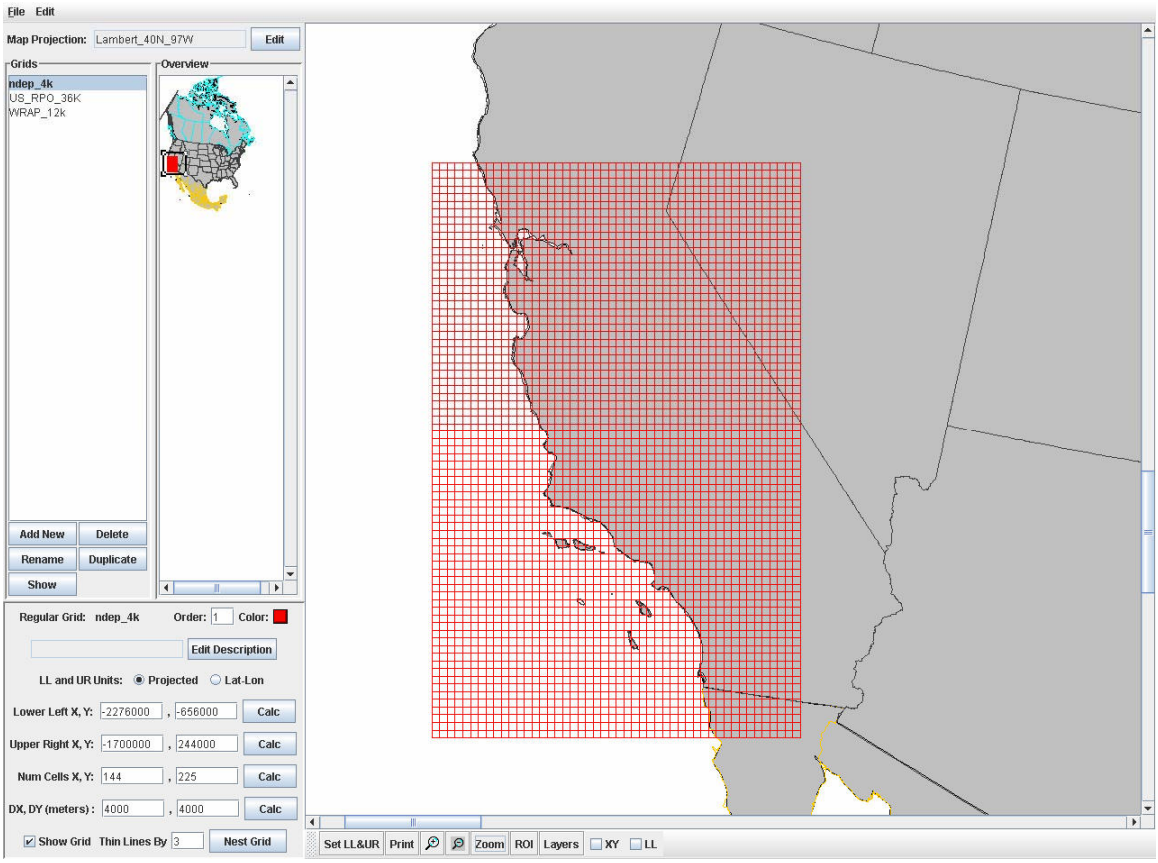


Figure C-1. 4-km grid resolution modeling domain to be used for the N deposition sensitivity studies in California for both CMAQ and CALPUFF

Table C-1. MM5, CMAQ, and CALPUFF vertical layer structure for the N-DEP 2002 application

MM5	CMAQ			CALPUFF	
4-km Layers	**Layers**	**Sigma**	**Height (m)**	**Layers**	**Height (m)**
19–top	19-top	0.000	14662		
18	18	0.250	8127		
17	17	0.450	5160		
16	16	0.600	3448	10–top	3000
15	15	0.700	2462	9	2200
14	14	0.770	1828		
13	13	0.820	1400	8	1500
12	12	0.860	1071	7	1000
11	11	0.880	911		
10	10	0.900	753		
9	9	0.920	598	6	600
8	8	0.940	445		
7	7	0.950	369		
6	6	0.960	294	5	300
5	5	0.970	220		
4	4	0.980	146	4	160
3	3	0.985	109		
2	2	0.990	73	3	80
1	1	0.995	36	2	40
				1	20
0 (ground)	0 (ground)	1.000	0	0 (ground)	0

1.1.4 Base Case

Meteorology

The raw 4-km MM5 output fields (described in Section 2) were post-processed with the CMAQ MCIP version 2.2 to produce base case, CMAQ-ready meteorological input files. The MCIP processor addresses issues related to data format translation, conversion of units of parameters, diagnostic estimations of parameters not provided, extraction of data for appropriate window domains, reconstruction of meteorological data on different vertical grid resolutions through collapsing or interpolation as needed, and to enforce consistency among the meteorological variables (Byun 1999a, 1999b).

The MCIP options selected in processing the MM5 files are (1) "pass-through" option where PBL values from the MM5 files were used; (2) radiation fields from MM5 files were used; and (3) RADM dry deposition routine was chosen to calculate dry deposition velocities. The CMAQ-ready files generated from the N-DEP 2002 MM5 run span the entire year.

Emissions

The CMAQ-ready emissions files are processed with the SMOKE emissions processor. Plume rises from point source emissions are calculated with plume-rise algorithm in SMOKE and the CMAQ-ready meteorological input fields. The plume rises heights are converted from heights above ground level into sigma levels. Point sources emissions rates are placed into the corresponding CMAQ sigma layers. Surface emission rates are added into layer one of the CMAQ-ready emissions files. The plume-rise calculation is a major difference between the CALPUFF and CMAQ models.

Ancillary Inputs

CMAQ requires several other types of input files, including initial/boundary conditions and photolysis rates. The initial and boundary conditions were generated with the standard CMAQ Initial Condition (ICON) and Boundary Condition (BCON) preprocessors. The initial concentration used in this study was generated from a time invariant set of vertical concentration profiles. After generating the CMAQ-ready initial concentration input file, the CMAQ simulation began on December 30, 2001, to allow two weeks of spin-up before the actual start of the annual simulation. Table C-2 contains a listing of six species (out of fifty-six species) in the time-invariant vertical initial concentration profile.

The CMAQ boundary conditions files are produced from another set of time invariant vertical concentration profile. The time-invariant boundary condition file was used throughout the annual simulation. Table C-3 contains a listing of six species (out of fifty-five species) in the time-invariant vertical boundary concentration profile.

The CMAQ JPROC processor was used to generate photolysis rates for the CMAQ runs. Ozone data from Total Ozone Mapping Spectrometer (TOMS) were downloaded from the Internet (http://jwocky.gsfc.nasa.gov/) for the entire year of 2002, to adjust the photolysis rates.

Table C-2. CMAQ predefined vertical profiles for initial condition (ppm)

σ-level	HNO_3	NH_3	NO	NO_2	O_3	PAN
0.20	0.00000088	0.00000387	8.8E-14	0.0000088	0.04	0
0.50	0.00000303	0.0000458	3.03E-13	0.0000303	0.04	0
0.648	0.00000854	0.000365	8.54E-13	0.0000854	0.04	0.000015
0.744	0.00000854	0.000365	8.54E-13	0.0000854	0.04	0.00005
0.808	0.00001	0.0005	1E-12	0.0001	0.04	0.00005
0.839	0.00001	0.0005	1E-12	0.0001	0.04	0.00005
0.868	0.00001	0.0005	1E-12	0.0001	0.04	0.00005
0.893	0.00001	0.0005	1E-12	0.0001	0.04	0.00005
0.916	0.00001	0.0005	1E-12	0.0001	0.04	0.00005
0.938	0.00001	0.0005	1E-12	0.0001	0.04	0.00005
0.956	0.00001	0.0005	1E-12	0.0001	0.04	0.0001
0.97	0.00001	0.0005	1E-12	0.0001	0.04	0.0001
0.98	0.00001	0.0005	1E-12	0.0001	0.04	0.0001
0.988	0.00001	0.0005	1E-12	0.0001	0.04	0.0001
0.995	0.00001	0.0005	1E-12	0.0001	0.04	0.0001
1.00	0.00001	0.0005	1E-12	0.0001	0.04	0.0001

Table C-3. CMAQ predefined vertical profiles for boundary condition (ppm)

σ-level	HNO_3	NH_3	NO	NO_2	O_3	PAN
0.30	0.0001	0.00001	0	0	0.07	0.000015
0.60	0.0002	0.00002	0	0	0.06	0.000015
0.84	0.0005	0.00002	0.000042	0.000084	0.05	0.000075
0.93	0.0005	0.00003	0.000083	0.000167	0.045	0.00015
0.98	0.0005	0.0001	0.000083	0.000167	0.04	0.00015
1.00	0.0005	0.0001	0.000083	0.000167	0.035	0.00015

1.1.5 CMAQ Modeling

CMAQ is being updated annually by the EPA and the version 4.4 released October, 2004 was used in this study. The CCTM simulations were performed on a 4-km resolution grid with 144 x 225 grid cells in each layer and 19 vertical layers extending from the ground to about 21,000 meters (13 miles) above sea level. The CMAQ system allow for a variety of choices for treating the numerical solution of the transport processes and chemistry. Table C-4 displays the scientific options used in the CMAQ simulations for both the base case and the sensitivity case.

For the base case, CMAQ chemistry-transport simulations were performed for the entire year of 2002. All CMAQ simulations were performed in UTC and the figures were all produced in UTC. The CMAQ simulations were performed on Linux-based workstations.

In the sensitivity case, the initial, boundary condition files, photolysis files, and meteorological input files remain the same. The only change was the addition of the Metcalf Energy Center into the daily emissions files. The Metcalf Energy Center is a

600 megawatt (MW), natural gas-fired, combined-cycle electricity generating plant located in San Jose, California.

The Annual total emissions for this source were 28 tons/yr VOC; 123.4 tons/yr NOx; 588 tons/yr CO; 10.6 tons/yr SO2; and 91.3 tons/yr PM2.5. The source location was latitude 37.2815 and longitude -121.9598. This was located in column 26 and row 165 of the modeling domain shown in Figure C-1. This source did not include NH3 emissions. The NOx emissions mass are calculated on an NO2 basis.

Table C-4. Model configurations for the CMAQ simulations

Model Option	CMAQ
Model Version	Version 4.4 (October 2004)
Horizontal Resolution	36/4 km
No. Vertical Layers	NZ = 19
Horizontal Advection	PPM
Vertical Advection	PPM
Horizontal Diffusion	Spatially Varying
Vertical Diffusion	K_V (Eddy Diffusion)
Minimum Vertical Diffusivity (1)	0.1 m^2/s
MM5 Configuration	Pleim-Xiu/ACM
MM5 Processing	MCIP2.2 Pass Through
Gas-Phase Chemistry	CB4
Gas-Phase Chemistry Solver	MEBI/Hertel
Secondary Organic Aerosol	SORGAM
Aqueous-Phase Chemistry	RADM
Aerosol Chemistry	AE3/ISORROPIA
Dry Deposition	Pleim-Xiu
Plume-in-Grid	Off
Initial Concentrations	From VISTAS 36km
Boundary Conditions	Fixed

1.2 CALPUFF

CALPUFF is a non-steady-state meteorological and air quality modeling system developed and distributed by Earth Tech, Inc. The model has been adopted by the EPA in its *Guideline on Air Quality Models* (http://support.lakes-environmental.com/Models/AppW/appw_01.pdf) as the preferred model for assessing long-range transport of pollutants and their impacts on Federal Class I areas and on a case-by-case basis for certain near-field applications involving complex meteorological conditions. The modeling system consists of three main components and a set of preprocessing and post-processing programs. The main components of the modeling system are: (1) CALMET (a diagnostic three-dimensional meteorological model), CALPUFF (an air quality dispersion model), and CALPOST (a post-processing package). Each of these programs has a GUI. In addition to these components, there are numerous

other processors that may be used to prepare geophysical (land use and terrain) data in many standard formats, meteorological data (surface, upper air, precipitation, and buoy data), and interfaces to other models such as the MM5, the National Centers for Environmental Prediction (NCEP) Eta model, and the RAMS meteorological model (http://www.src.com/calpuff/calpuff1.htm).

This section describes how the CALPUFF modeling system was set up for this project. In setting up the model inputs, to the extent possible, the research team relied rely on the default values provided by the developers, to test how the out-of-the-box model compared to CMAQ. The PST time zone was used in the CALPUFF simulations.

1.2.1 CALMET (and CALMM5)

CALMET is a meteorological model that develops hourly wind and temperature fields on a three-dimensional gridded modeling domain. Associated two-dimensional fields such as mixing height, surface characteristics, and dispersion properties are also included in the CALMET outputs. This project used the CALMET option, which allows wind fields produced by MM5 to be used as an initial guess field as part of the CALMET objective analysis procedure. The interface program CALMM5 was used to convert the MM5 data into a form compatible with CALMET.

The CALMM5 interface program reads the MM5 v.2 data. As mentioned in Section 2, the latest available MM5 (v3.6.3) was used to produce the raw meteorological fields. Because the MM5 development team changed the output file format beginning at MM5 v.3, it was first necessary to run the utility program "v32v2," to convert MM5 v.3 format to v.2 format prior to running CALMM5 ("v32v2" is available at the NCAR/MM5 website: ftp://ftp.ucar.edu/mesouser/MM5V3/Util).

CALMM5 reads and interprets all information contained in the MM5 header. It also outputs horizontal and vertical velocity components, pressure, temperature, relative humidity, and vapor, cloud, rain, snow, ice, and graupel mixing ratios into CALMET-ready format. Because the Lambert conformal projection was used, CALMM5 converts the MM5 north-south and east-west components (U, V) of wind velocities back to wind speed and wind direction with respect to true north.

In setting up the CALMM5 runs, the project team created an automated script to read in the 2002 raw MM5 outputs in 25-hour segments, and created a total of 365 CALMM5 output files for the entire year. The starting and ending date/hour was shifted from UTC to PST so the CALMM5 outputs would begin from 00 PST of the first day and end in 00 PST of the next day.

Prior to running CALMET, the team had to create the GEO.DAT file, which contains the geophysical data inputs required by the CALMET model. The inputs include land use type, elevation, surface parameters (surface roughness length, albedo, Bowen ratio, soil heat flux parameter, and vegetation leaf area index), and anthropogenic heat flux. Instead of using the standard utility programs provided by CALPUFF modeling system, the team wrote a separate program to read in the data directly from MM5 TERRAIN file to create GEO.DAT.

After processing raw MM5 data with CALMM5 and create GEO.DAT, the next step was to create the CALMET.INP file which contains the data that define a particular model run and model option flags. The research team set up CALMET to use gridded prognostic model outputs from MM5. Some of the CALMET model options used are tabulated in Table C-5.

After running CALMET for the entire year of 2002, three hundred and sixty five "CALMET.DAT" files were created. These files contain the meteorological data fields, terrain elevations, surface roughness lengths, and land-use types used by the CALPUFF air quality model.

Table C-5. CALMET model options used in the N-DEP simulations

Input Group	Option	Description
0	MM5.DAT	MM5 data file from CALMM5
	No upper air file used	
	No overwater station used	
1	IBTZ = 8	PST used in the simulations
	IRLG = 25	25 hours included in each day
2	PMAP = LCC	Lambert Conformal Conic Projection (LCP)
	RLAT0 = 40.0 N	Origin latitude in LCP
	RLON0 = 97.0 W	Reference longitude in LCP
	XLAT1 = 33.0 N	Latitude of the two standard LCP parallels
	XLAT2 = 45.0 N	
	NX = 144	Number of columns
	NY = 225	Number of rows
	XORIGKM = -2276.00	Reference X coordinate (km) of the southwest corner of grid cell (1,1)
	YORIGKM = -656.00	Reference Y coordinate (km) of the southwest corner of grid cell (1,1)
	NZ = 10	Number of vertical levels
4	NOOBS = 2	Use MM5 for surface, overwater, and upper air data
	ICLOUD = 3	Gridded cloud cover from Prognostic relative humidity (R.H.)
5	IEXTRP = 1	No extrapolation for surface wind observation
6	ITPROG = 2	3-D data from MM5

1.2.2 CALPUFF

CALPUFF is a non-steady-state, Lagrangian, Gaussian puff model containing modules for complex terrain effects, overwater transport, costal interaction effects, building downwash, wet and dry removal, and simple chemical transformation (Scire et al. 2000).

CALPUFF is capable of computing dry deposition rates of gases and particulates as a function of geophysical parameters, meteorological conditions, and pollutants species

through a full resistance model. An empirical scavenging coefficient approach is also included to compute the depletion and wet deposition fluxes due to precipitation scavenging.

Similar to CALMET runs, all CALPUFF runs use as much default values as possible. Some of the CALPUFF options are tabulated in Table C-6.

The CALPUFF model allows point source emissions to be released either at a constant rate or with arbitrarily varying emissions. The constant rate option was used in all of this project's CALPUFF simulations. Because part of this project was to compare N deposition between CMAQ and CALPUFF, the research team had to make sure total emissions released during the comparison period were identical. Table C-7 tabulates the January and July emissions that were used in CMAQ simulations. The CALPUFF emission rates for the four emitted species were calculated based upon these values. A stack height of 145 ft (44 meters, m) was obtained from the Metcalf Energy Center website. Stack height (3 m, or 10 ft), exit velocity (14.3 meters per second (m/s), or 47 ft/s), and exit temperature (404°K, or 268°F) were taken from SMOKE defaults so the simulation results could be as similar to CMAQ as possible.

Table C-6. CALPUFF model options used in the N-DEP simulations

Input Group	Option	Description
0	Ozone data	Hourly ambient ozone measurements from EPA Air Quality System (AQS) in the N-DEP domain were used
	NMETDAT = 31	31 days are used per run
1	XBTZ = 8	Base time zone: PST
	IRLG = 744	Total length of run = 744 hours
	NSPEC = 7	7 chemical species
	NSE = 4	4 species emitted
2	MCHEM = 3	Transformation rates computed internally
3	SO_2, SO_4, NO, NO_2, HNO_3, NO_3, PM_{10}	Species modeled
4	NX = 144	No. X grid cells
	NY = 225	No. Y grid cells
	NZ = 10	No. vertical layers
11	MOZ = 1	Hourly ozone concentration file from OZONE.DAT
13b	X coord = -2174.00 km	
	Y coord = 2.0 km	
	Stack height = 44.196 m	
	Stack diameter = 5.486 m	
	Exit vel. = 19.1 m/s	
	Bldg. Dwash = 0	
	SO_2 =	Emissions rate
	SO_4 =	

Input Group	Option	Description
	NO =	
	NO_2 =	
	HNO_3 =	
	NO_3 =	
	PM_{10} =	

Table C-7. CALPUFF January and July emissions rates for the four emitted species

		January		July	
	Short_ton/year	g/s	kg/month	g/s	kg/month
NO	111.06	2.59	6938.01	3.83	10256.19
NO_2	12.34	0.29	770.89	0.43	1139.58
SO_2	10.6	0.25	662.19	0.37	978.89
PM_{10}	91.3	2.13	5703.59	3.15	8431.39

1.3 Ambient Monitoring Data for Model Validation

The project team compiled the ground-level model evaluation database for 2002, using several routine and research-grade ambient monitoring databases including the following for fine particulate matter:

- Interagency Monitoring of Protected Visual Environments (IMPROVE)
- Clean Air Status and Trends Network (CASTNET)
- EPA Speciation Trends Network (STN)
- National Atmospheric Deposition Program (NADP)
- Southeastern Aerosol Research and Characterization (SEARCH).

In addition, the project used the EPA's Aerometric Information Retrieval System (AIRS/AQS) database for routine gas-phase concentration measurements for archived ozone, NO, NO_2, and CO.

Data from these ambient networks are briefly described in the following sections. Model evaluation was performed by comparing model predictions to ambient data. Model evaluation software developed by the University of California at Riverside (UCR) was used to evaluate the CMAQ model results. This software generates tables of statistical measures, scatter plots, and time series plots. The UCR performance evaluation software is capable of producing more than 16 statistical measures. Illustrative results are included below, and additional plots are available on the UCR NDEP modeling website at: http://pah.cert.ucr.edu/aqm/ndep.

Figure C-2 displays the locations of the monitors for the various monitoring networks operating during 2002. Typically, these networks provide ozone, PM, and visibility measurements, and the types of data available from these specialized PM monitoring programs are summarized in Table C-8. Because of different lumping schemes in the model chemistry and the way model outputs in concentration units, some measured species cannot be compared directly to the model species. Certain mapping schemes are thus applied for model-to-observation species comparisons.

Table C-8. Summary of ambient databases used in the evaluation

Monitoring Network	Chemical Species Measured	Sampling Frequency; Duration	Data Availability (sites)
The Interagency Monitoring of Protected Visual Environments (IMPROVE)	Speciated $PM_{2.5}$ and PM_{10}	1 in 3 days; 24 hr	~62
Clean Air Status and Trends Network (CASTNET)	Speciated $PM_{2.5}$, Ozone	Weekly; Week	~72
EPA Air Quality System (AQS)	O_3, CO, SO_2, NO, NOy	Hourly; 1-hr average	~1536
Speciation Trend Network (STN)	Speciated $PM_{2.5}$	Varies; Varies	~215
National Acid Deposition Network (NADP)	WSO_4, WNO_3, WNH_4	Weekly	~100
Southeastern Aerosol Research and Characterization (SEARCH)	$PM_{2.5}$ (OC, BC, SO_4, NO_3, NH_4, Elem.); O_3, NO, NO_2, NOy, HNO_3, SO_2, CO, NH_3)	Hourly, Daily; varies	8

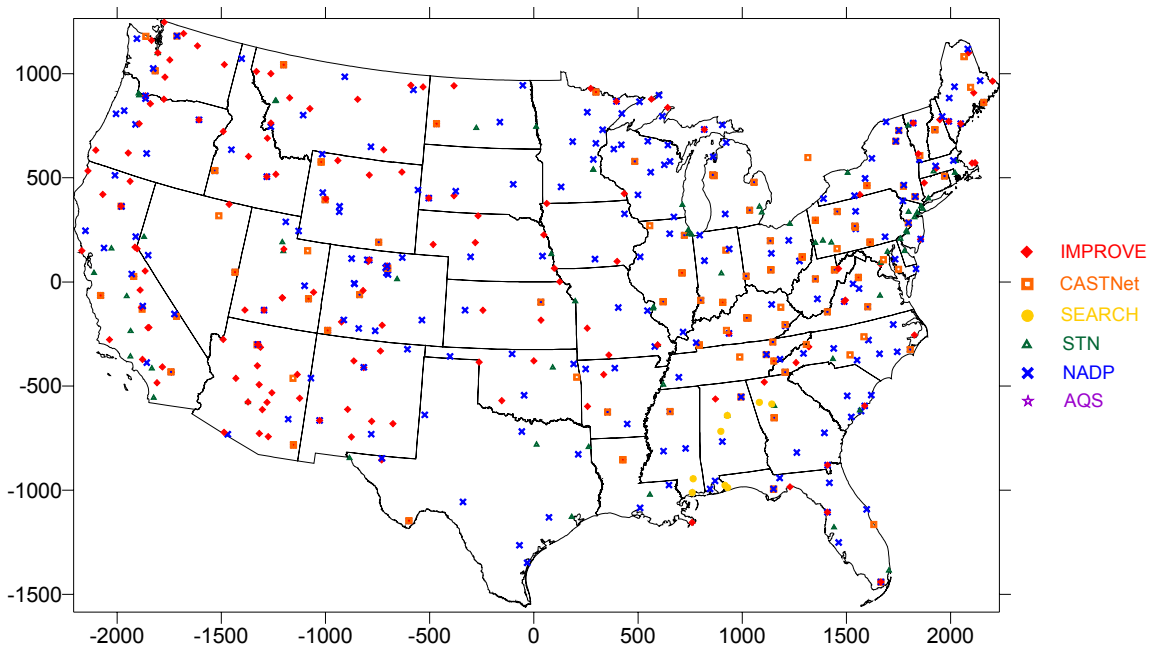


Figure C-2 Location of the monitors for the various monitoring networks (IMPROVE, CASTNET, SEARCH, STN, NADP, and AQS) operating during 2002

1.4 Summary of the Monitoring Networks

1.4.1 IMPROVE

The Interagency Monitoring of Protected Visual Environments monitoring network (http://vista.cira.colostate.edu/improve) reports detailed chemical species in its measurements of major visibility-reducing aerosol species on a twice-a-week basis. The PM fine mass species being used in the evaluation are as follows:

- Sulfates (SO_4), as sulfate ion
- Nitrates (NO_3), as nitrate ion
- Organic carbon (OC), as organic carbon mass
- Elemental carbon (EC), as light absorbing carbon or carbon soot;
- Soil (SOIL), as fine soil and is sum of several inorganic elements such as Al, Si, Ca, Fe and Ti.

These species are all measured using a 2.5-micron cut point inlet. The IMPROVE monitors also measure total PM_{10} and $PM_{2.5}$ mass. These values are reported as the fine matter (FM) portion of the mass ($PM_{2.5}$), and the coarse matter (CM) portion of the mass, (PM_{10}–$PM_{2.5}$). In CMAQ, water as fine particle species is not included among the mapping of IMPROVE species, because IMPROVE measures only dry particles. In addition, IMPROVE defines SOIL as fine soil concentration, which is the sum concentrations of several inorganic species. Although fine soil is not specifically defined in CMAQ, it is taken as unspeciated portion of $PM_{2.5}$ emitted species. Therefore, the CMAQ model species A25 is used as surrogate for IMPROVE's fine soil concentration.

Figures C-3 and C-4 show time-series plots for NH_4 and aerosol nitrate concentrations at IMPROVE sites (Joshua Tree, Pinnacle Forest, and Yosemite) versus CMAQ WRAP 36-km and CMAQ 4-km California Nitrogen Deposition base case simulation results for the entire year of 2002.

1.4.2 CASTNET

The Clean Air Status and Trends Network (CASTNET) was developed to monitor dry acidic deposition and rural ground level ozone. It includes measurements of ambient concentrations and meteorology and land use, which are used to calculate dry deposition rates. A majority of the CASTNET sites measure sulfate and nitrate, including both gaseous (as HNO_3) and aerosol phases, and ammonium in seven-day filter samples. Detailed data collection procedures are described at the EPA CASTNET website: http://www.eap.gov/castnet.

In short, atmospheric concentration data are collected at each site with open-faced, three-stage filter packs. The filter pack contains a Teflon filter for collection of particulate species, a nylon filter for nitric acid, and a base-impregnated cellulose (Whatman) filter for sulfur dioxide. Filter packs are exposed for one-week intervals, and are later extracted and analyzed for certain species.

Because CASTNET reports gaseous species such as SO_2 and HNO_3 in micrograms per square meter ($\mu g/m^3$) units, and all other models (except REMSAD) have gaseous species in parts per million by volume (ppmV) units, conversion factors (assumed under standard conditions for temperature and pressure (STP) of 2617.6 and 2576.7 are applied for the modeled SO_2 and HNO_3 species. It has been suggested that total nitrate (NO_3 + HNO_3)—instead of individual aerosol nitrate and gaseous nitric acid—should be used for observation-modeled comparison, because of the possible volatilization loss on the Teflon filter pack used in CASTNET (Ames and Malm 2001). Notice that a ratio of 0.9841, molecular weight ratio of NO_3/HNO_3, is applied in CASTNET's total nitrate calculation.

Figures C-5 and C-6 show time-series plots for nitric acid and NH_4 concentrations at CASTNET sites (Joshua Tree, Pinnacle Forest, and Yosemite) versus CMAQ WRAP 36-km and CMAQ 4-km California Nitrogen Deposition base case simulation results for the entire year of 2002.

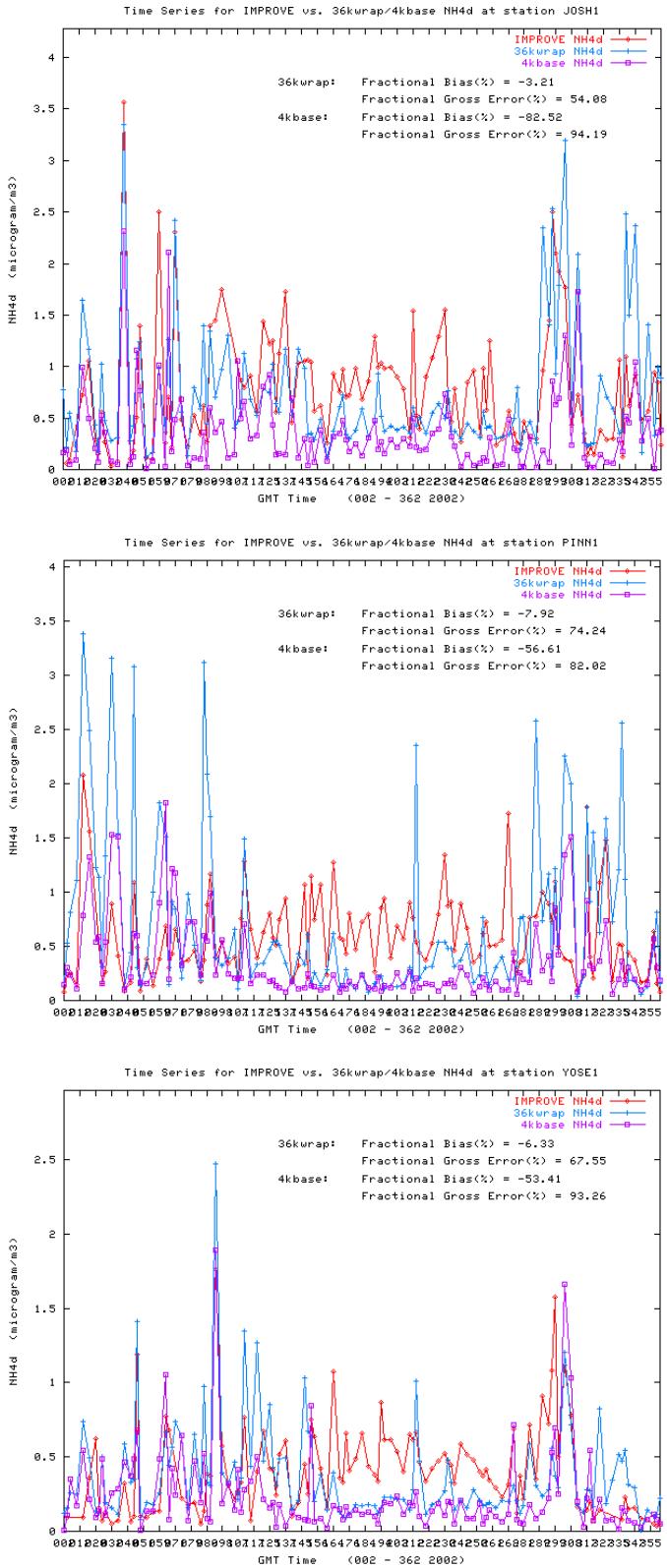


Figure C-3. Time-series plots for NH_4 concentration at IMPROVE sites (Joshua Tree, Pinnacle Forest, and Yosemite) versus CMAQ WRAP 36-km and CMAQ 4-km California Nitrogen Deposition simulation results for entire year of 2002

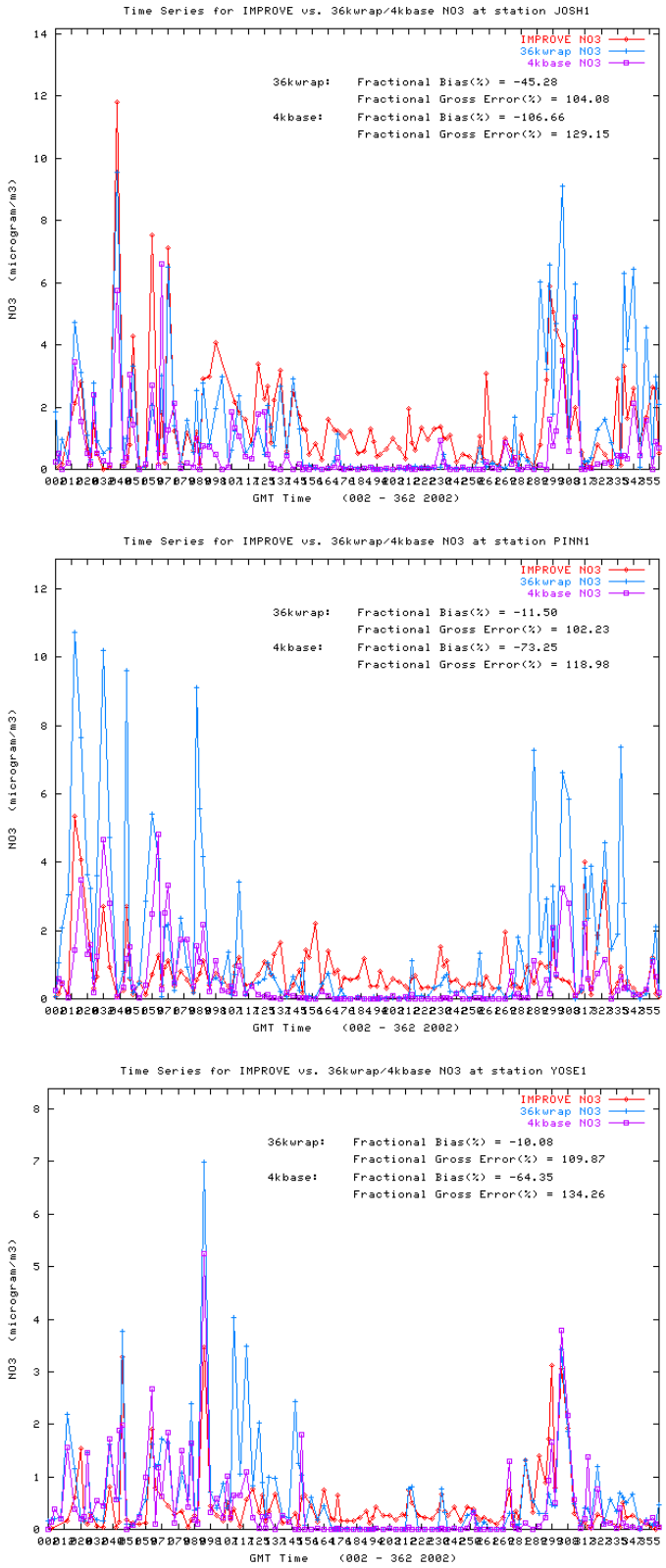


Figure C-4. Time-series plots for aerosol nitrate concentration at IMPROVE sites (Joshua Tree, Pinnacle Forest, and Yosemite) versus CMAQ WRAP 36-km and CMAQ 4-km California Nitrogen Deposition simulation results for entire year of 2002

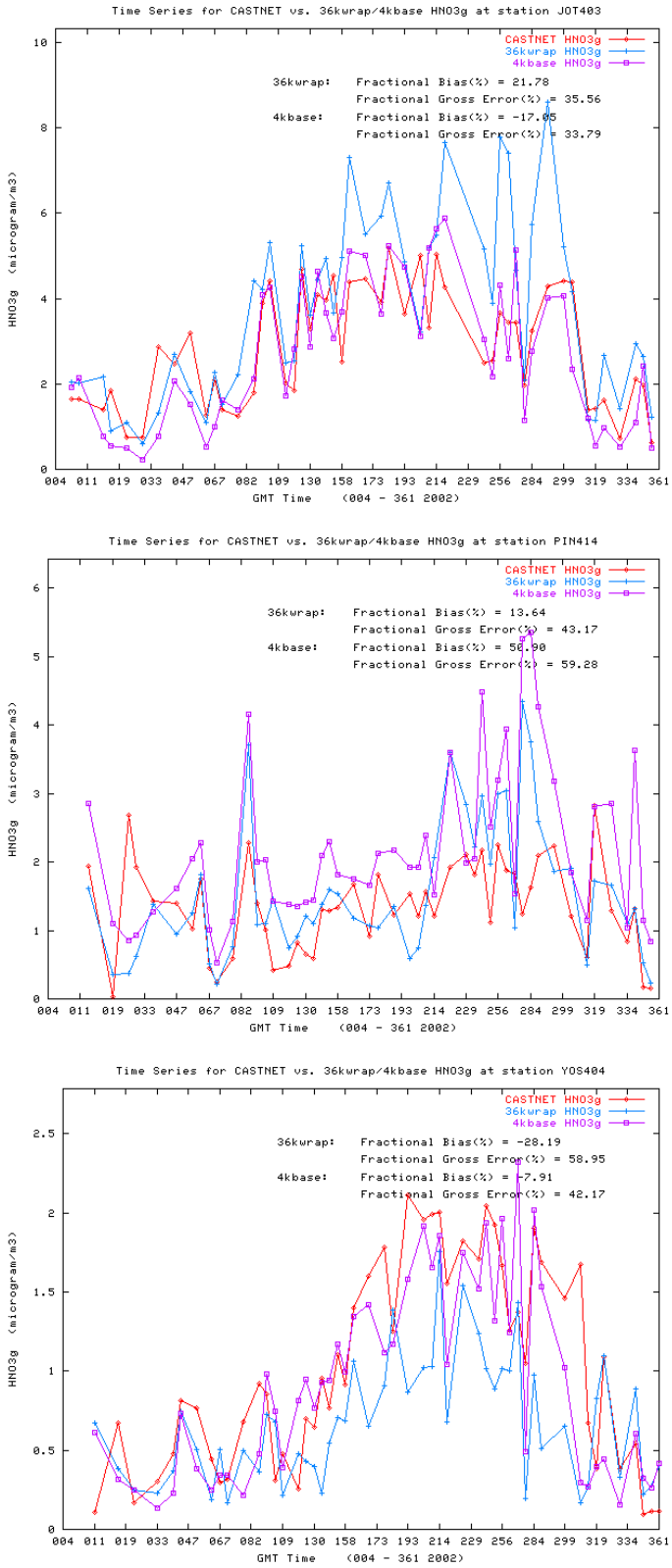


Figure C-5. Time-series plots for nitric acid concentration at CASTNET sites (Joshua Tree, Pinnacle Forest, and Yosemite) versus CMAQ WRAP 36-km and CMAQ 4-km California Nitrogen Deposition simulation results for entire year of 2002

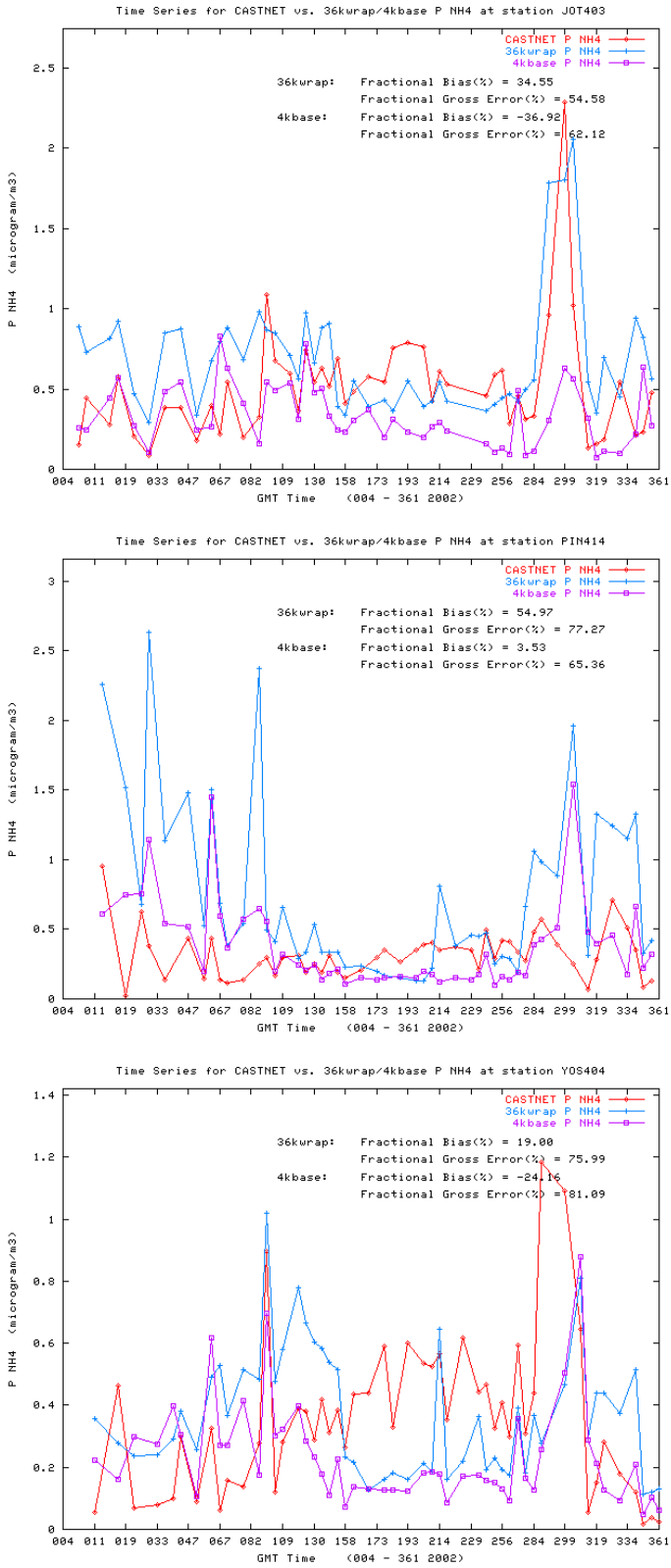


Figure C-6. Time-series plots for NH_4 concentrations at CASTNET sites (Joshua Tree, Pinnacle Forest, and Yosemite) versus CMAQ WRAP 36-km and CMAQ 4-km California Nitrogen Deposition simulation results for entire year of 2002

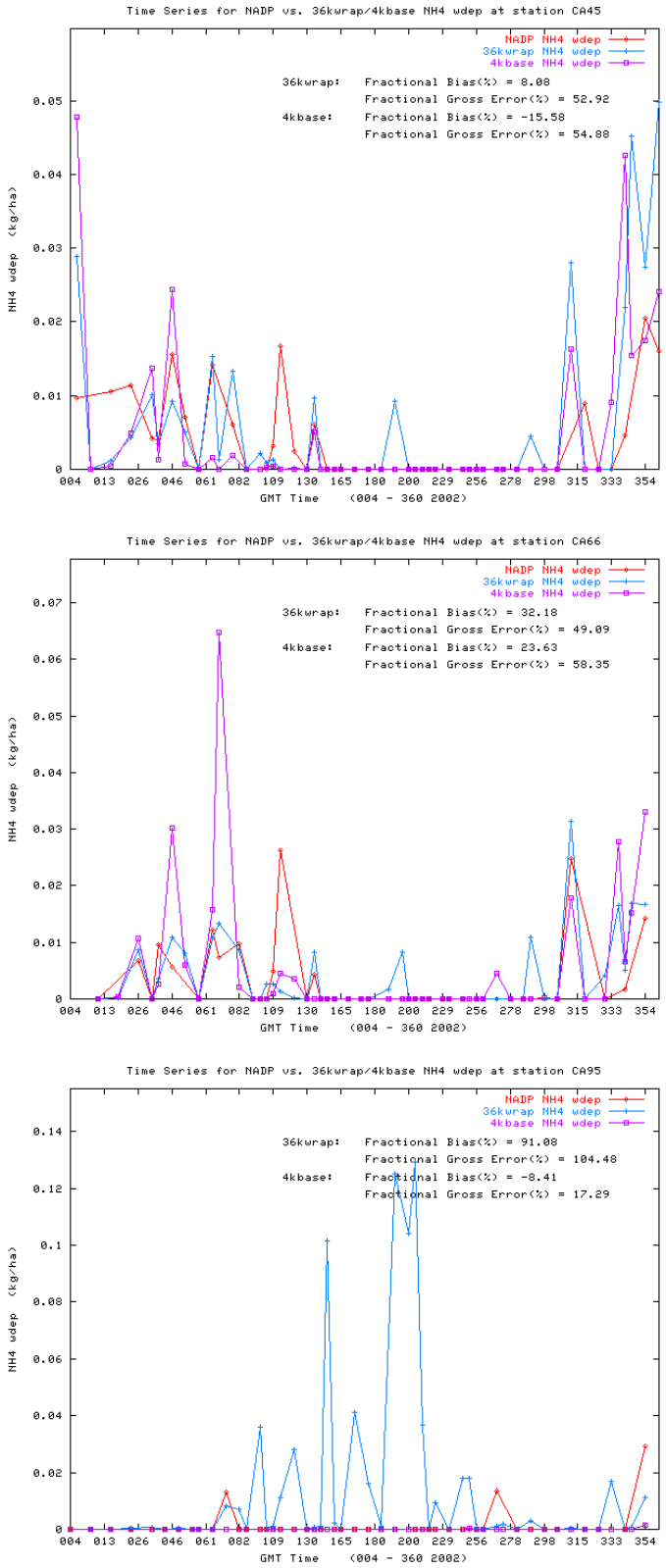


Figure C-7. Time-series plots for NH_4 wet deposition at three California NADP sites versus CMAQ WRAP 36-km and CMAQ 4-km California Nitrogen Deposition simulation results

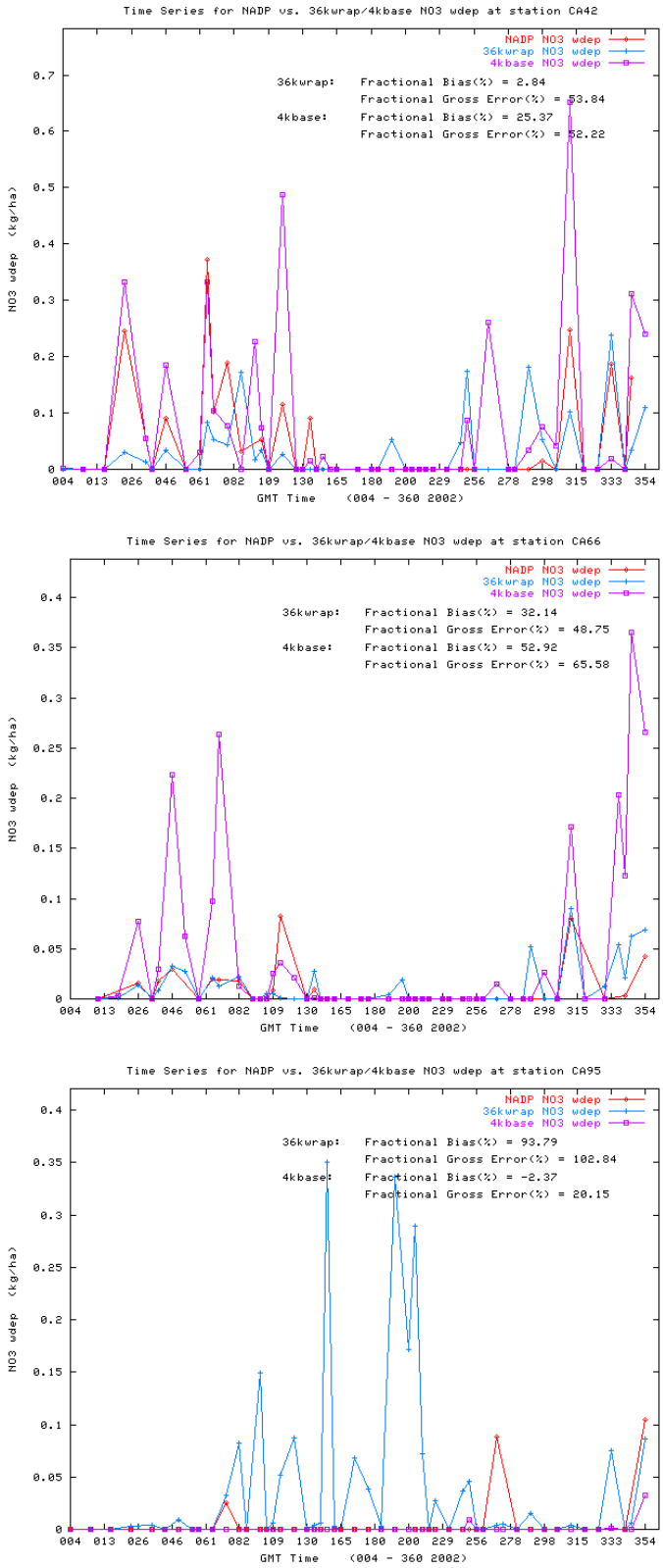


Figure C-8. Time-series plots for aerosol nitrate wet deposition at three California NADP sites versus CMAQ WRAP 36-km and CMAQ 4-km California Nitrogen Deposition simulation results

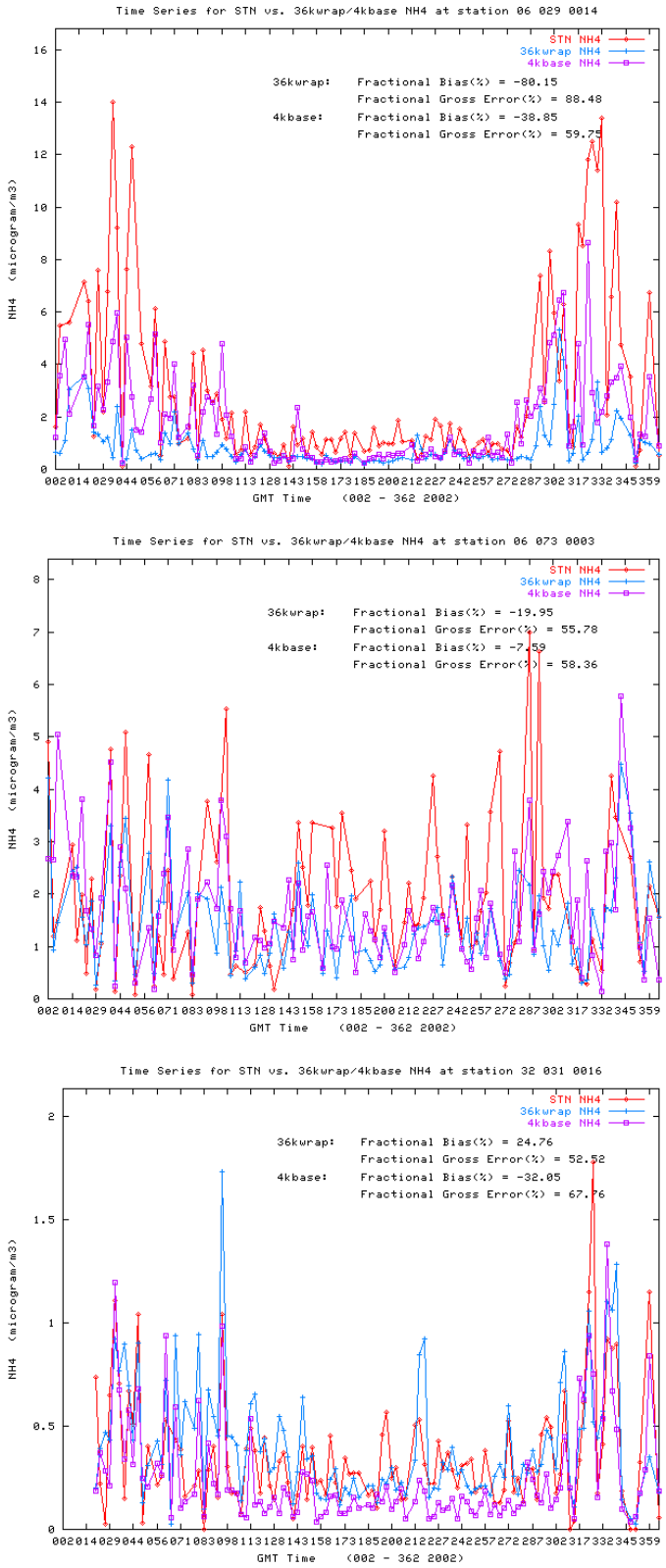


Figure C-9. Time-series plots for NH_4 concentration at three California STN sites versus CMAQ WRAP 36-km and CMAQ 4-km California Nitrogen Deposition simulation results

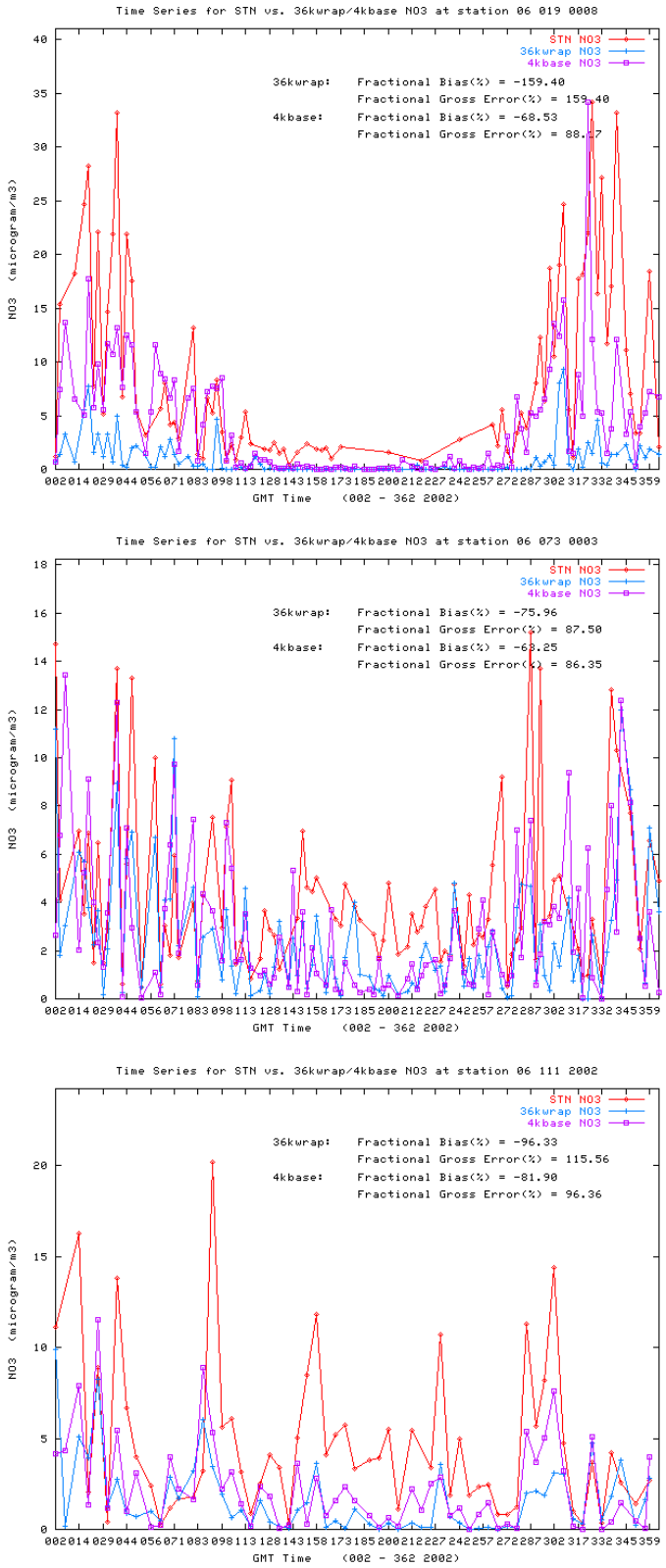


Figure C-10. Time-series plots for aerosol nitrate concentration at three California STN sites versus CMAQ WRAP 36-km and CMAQ 4-km California Nitrogen Deposition simulation results

1.4.3 AQS

The Air Quality System database is EPA's repository of "criteria air pollutant"— carbon monoxide (CO), nitrogen dioxide (NO_2), sulfur dioxide (SO_2), ozone (O_3), particulate matter (PM_{10} and $PM_{2.5}$), and lead (Pb) monitoring data since the 1970s. It replaced the Aeronomic Information Retrieval System (AIRS) as the EPA's main repository for ambient air monitoring data, including data from the State and Local Air Monitoring Stations (SLAMS), the National Air Monitoring Stations (NAMS), Photochemical Assessment Monitoring Stations (PAMS), and other data sources. A majority of the ozone (and several gaseous components, including SO_2, CO, NO_2, and others), can be retrieved for hourly data from the EPA's Air Quality System (AQS) web-site: www.epa.gov/ttn/airs/airsaqs/archived%20data/downloadaqsdata.htm through data query requests. In this study, only hourly gaseous species in AQS were used for model evaluations. Unlike CASTNET data, gaseous species in AQS are reported in ppmV units.

1.4.4 NADP

The National Atmospheric Deposition Program/National Trends Network (NADP/NTN) is designed to measure wet deposition. The network is a cooperative effort between State Agricultural Experiment Stations, the U.S. Geological Survey, U.S. Department of Agriculture, and other governmental and private entities. It includes over 200 sites in the continental United States, Alaska, Puerto Rico, and the Virgin Islands. The purpose of the network is to collect data on the chemistry of precipitation for monitoring of geographical and temporal long-term trends. The precipitation at each station is collected weekly, and is analyzed for hydrogen (acidity as pH), sulfate, nitrate, ammonium, chloride, and base cations (such as calcium, magnesium, potassium, and sodium). The NADP network includes a quality assurance program, so the research team expects to use these data without any additional QA. Figures C-7 and C-8 show time-series plots for NH_4 and aerosol nitrate wet deposition at three California NADP sites versus CMAQ WRAP 36-km and CMAQ 4-km California Nitrogen Deposition simulation results for the entire year of 2002.

The NADP includes the Mercury Deposition Network (MDN) and the Atmospheric Integrated Research Monitoring Network (AIRMoN), designed to study precipitation chemistry trends with greater temporal resolution. Precipitation samples are collected daily from a network of nine sites and analyzed for the same constituents as the NADP/NTN samples. The research team is currently investigating the availability of the NADP and AIRMoN data; at present, the team has not been able to access these data.

1.4.5 STN

EPA's Speciation Trends Network includes about 215 monitoring stations nationwide. It appears that among these 215 sites may include IMPROVE sites or other data from other networks. This, however, needs to be verified. Daily $PM_{2.5}$ data are measured for 64 species in the STN network. Some archived STN data files were obtained from the EPA website: www.epa.gov/ttn/airs/airsaqs/archived%20data/archivedaqsdata.htm.

Figures C-9 and C-10 show time-series plots for NH_4 and aerosol nitrate concentrations at three California NADP sites versus CMAQ WRAP 36-km and CMAQ 4-km California Nitrogen Deposition simulation results for the entire year of 2002.

1.4.6 Model Performance Metrics

Statistical measures that are frequently used in current PM and visibility model performance evaluation include accuracy, error and bias. The calculations of error and bias statistic measures are based on the residuals of all pairs of model estimates and observations. Both error and bias measures provide a useful basis for comparison among model simulations across different model episodes. Although most model performance evaluations have used the observations to normalize the error and the bias, this approach can lead to misleading conclusions. When normalizing to very low observed concentration values (e.g., clean conditions) model over-predictions are weighted much more strongly than equivalent under-predictions, as suggested by Seigneur et al. (2000). Seigneur et al. (2000) recommended that peak bias, average fractional bias, average fractional gross error, and regression be included as the key statistics in model's operational evaluation to alleviate such problems. The statistical measures have been computed and are available upon request.

1.5 Results of Model Simulations

We present here selected results from the CALPUFF model showing the modeled deposition at different intervals in the model simulation.

Figures C-11 to C-14 show July 11 and 12 simulation results from CALPUFF and CMAQ models. These two days were chosen to demonstrate a more stagnant case in July. These model results are shown side by side to illustrate differences in deposition patterns from the two models. A larger amount of emissions were deposited close to the Metcalf power plant. Some parts of the emissions were also transported out of the northern boundary of the modeling domain. The color scale for CALPUFF ranges from 0.0 to 0.001 g-N/ha for CALPUFF and -0.01 to 0.01 g-N/ha for CMAQ.

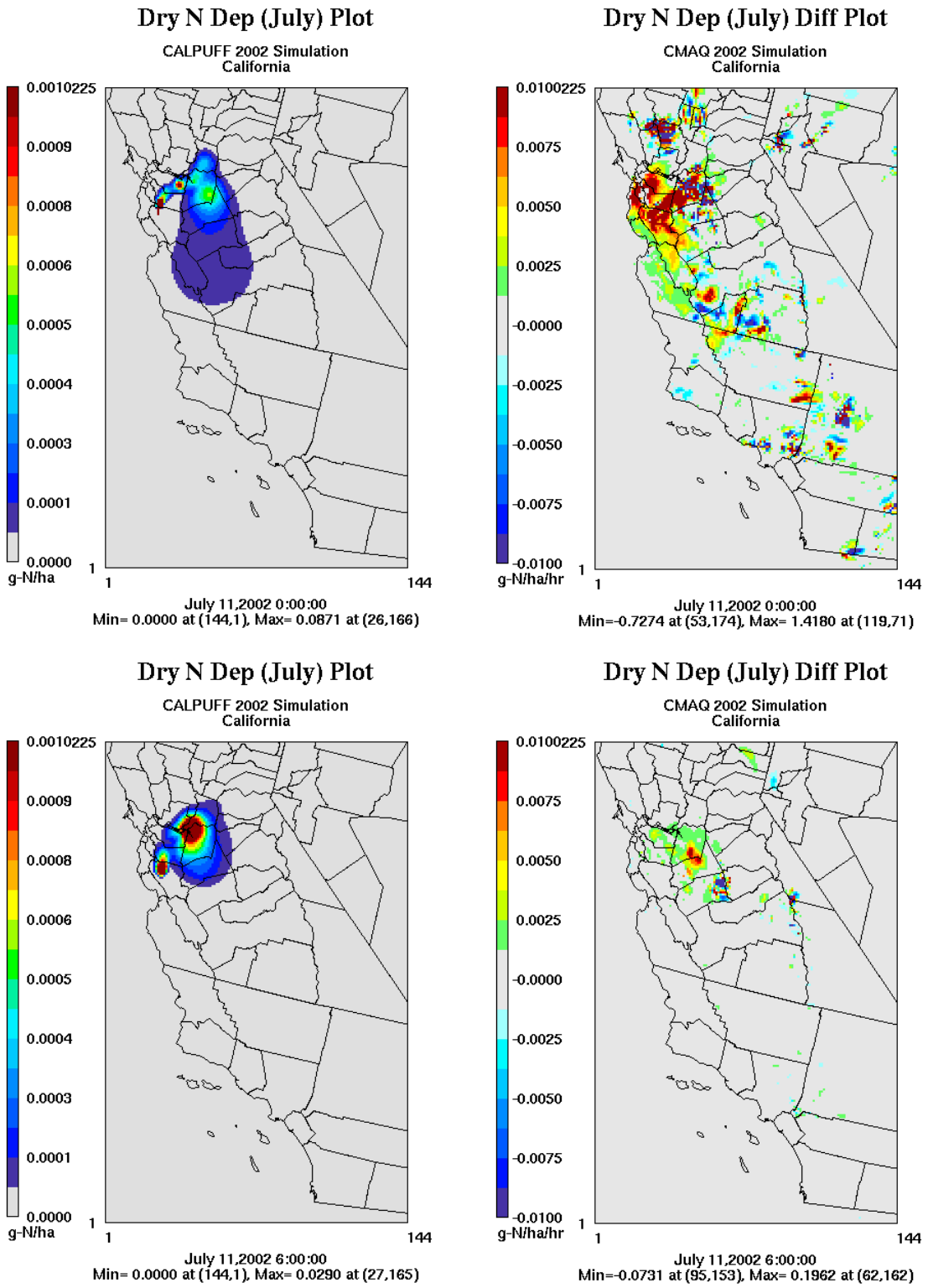


Figure C-11. CALPUFF versus CMAQ July 11, 2002 N dry deposition from the sensitivity case, with color scale from 0.0 to 0.001 g-N/ha for Calpuff and -0.01 to 0.01 g-N/ha for CMAQ

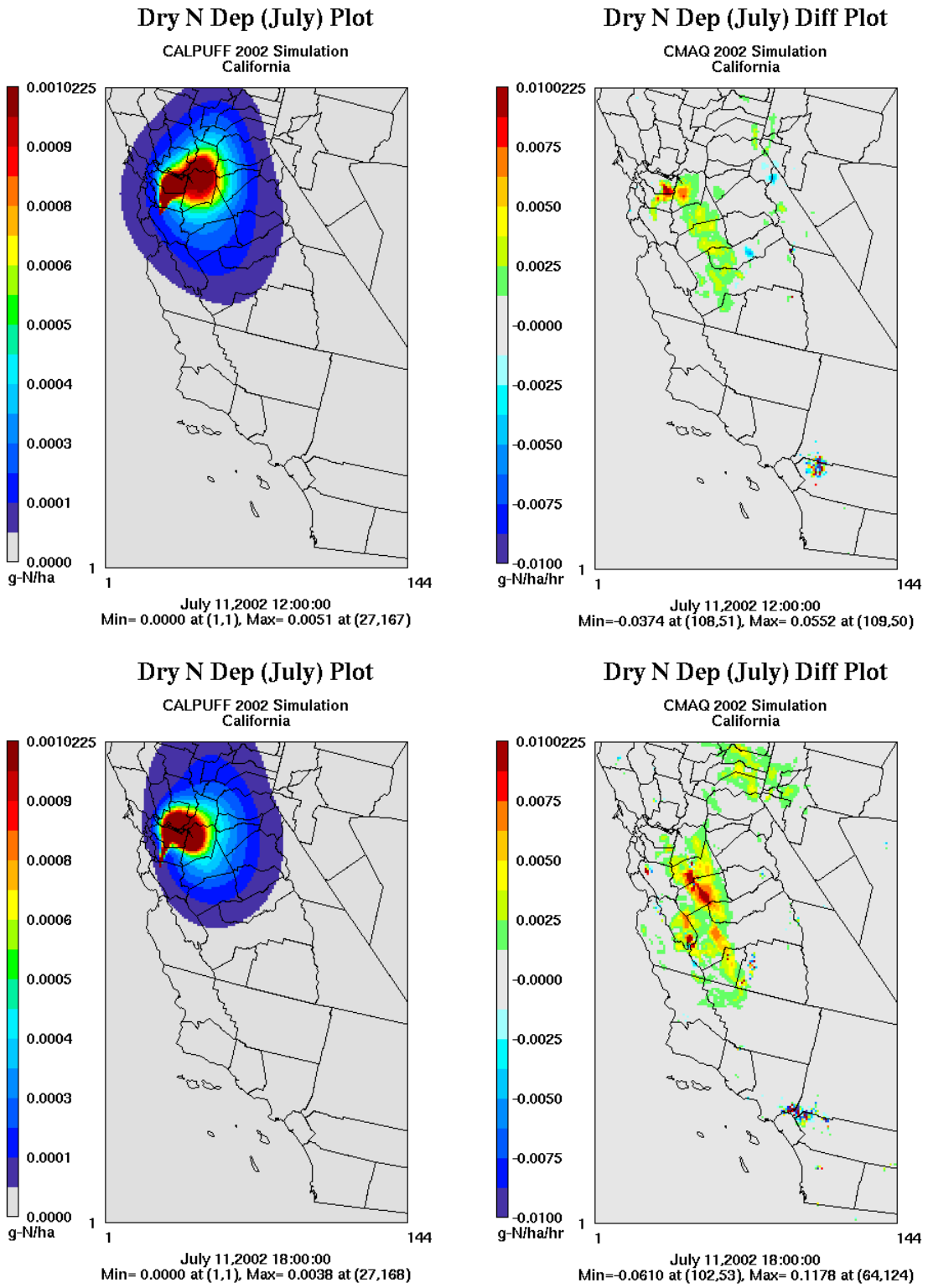


Figure C-12. CALPUFF versus CMAQ July 11, 2002 N dry deposition from the sensitivity case, with color scale from 0.0 to 0.001 g-N/ha for Calpuff and -0.01 to 0.01 g-N/ha for CMAQ

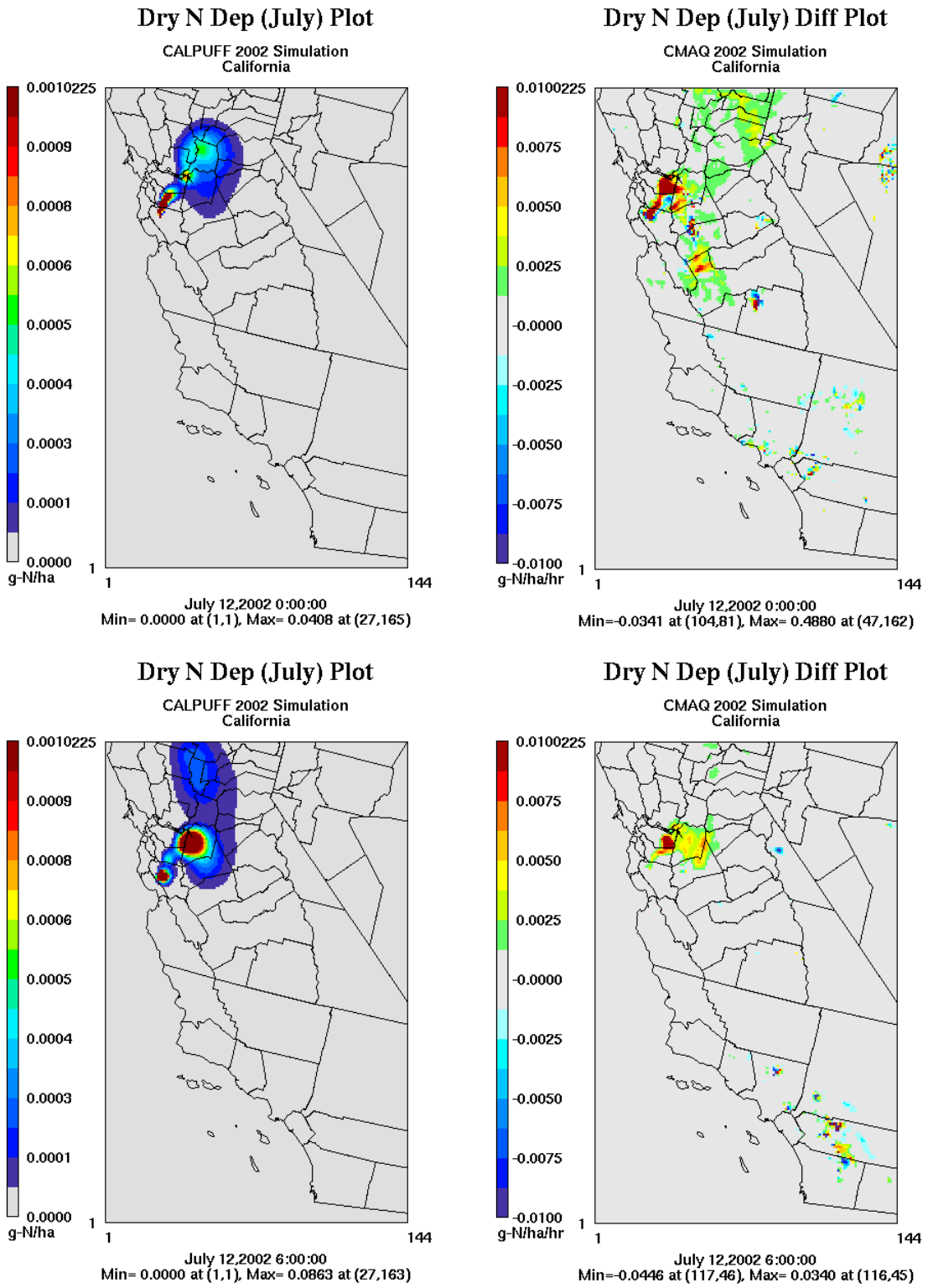


Figure C-13. CALPUFF versus CMAQ July 12, 2002 N dry deposition from the sensitivity case, with color scale from 0.0 to 0.001 g-N/ha for Calpuff and -0.01 to 0.01 g-N/ha for CMAQ

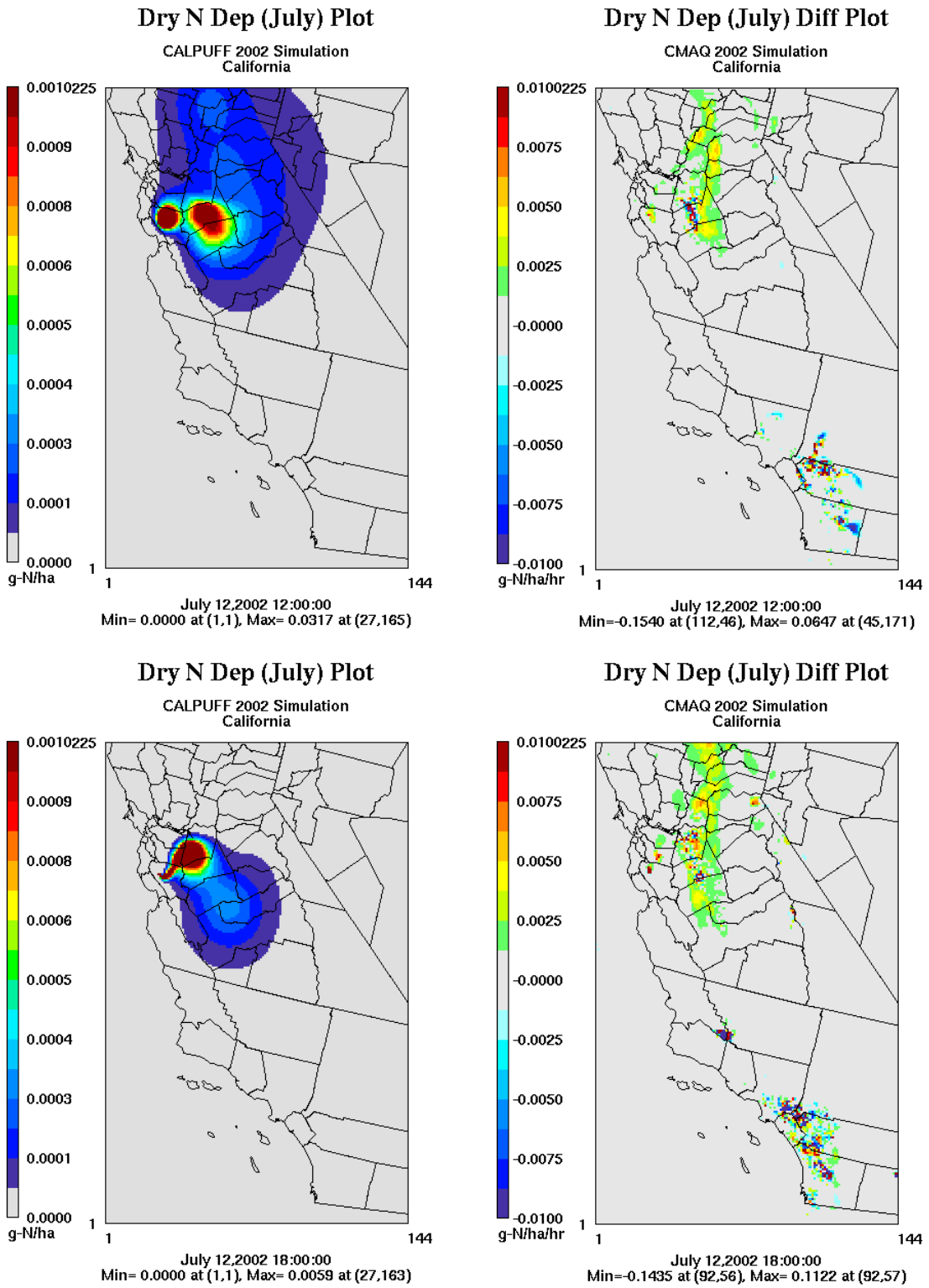


Figure C-14. CALPUFF versus CMAQ July 12, 2002 N dry deposition from the sensitivity case, with color scale from 0.0 to 0.001 g-N/ha for Calpuff and -0.01 to 0.01 g-N/ha for CMAQ