**Revised Ozone Modeling Protocol**

# AIR QUALITY MODELING ANALYSIS FOR THE DENVER EARLY ACTION OZONE COMPACT: Modeling Protocol, Episode Selection, and Domain Definition

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21 May 2003

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# 1.0 INTRODUCTION

The Denver metropolitan area has volunteered to participate in the U.S. Environmental Protection Agency's (EPA) Early Action Compact (EAC) Protocol process for the purpose of deferring the effective date of a nonattainment designation for the Denver area if a violation of the 8-hour ozone NAAQS occurs in the future. The lead agency in this EAC Protocol process is the Denver Regional Air Quality Council (RAQC). Providing assistance to the RAQC are the Colorado Department of Public Health and Environment (CDPHE), Denver Regional Council of Governments (DRCOG), and Colorado Department of Transportation (CDOT). ENVIRON International Corporation (ENVIRON) and it's subcontractor Alpine Geophysics, LLC (Alpine) has been retained to provide technical assistance to the RAQC and CDPHE in order to meet the technical milestones for emission inventory and photochemical modeling needed to fulfill the requirements of the Early Actions Ozone Compact for the Denver area.

## 1.1 Overview of the EAC Process

The EAC Protocol process (Cooke, 2002) requires a photochemical dispersion modeling demonstration to show attainment of the 8-hour ozone standard by December 2007. Any controls necessary are to be implemented by 2005. Development of credible photochemical dispersion modeling, an essential component of the EAC process, will be performed by the ENVIRON/Alpine science team in close cooperation with the technical staff of the RAQC and CDPHE. Key elements of the modeling analyses are described in this protocol document. The basic principals of the EAC Protocol are as follows:

> Early emission reductions to attain the 8-hour ozone standard;

> Local control, with broad-based public input;

> State support to ensure technical integrity of the early action plan;

> Early action plan incorporated into the SIP;

> Effective date of nonattainment designation and/or designation requirements is deferred (as long as all EAC terms and milestones are met);

> Safeguards to return to a traditional SIP requirements if EAC terms and/or milestones are not met.

In order to qualify for an EAC, an area must currently be attaining the 1-hour ozone standard. If a current 1-hour ozone attainment area has 8-hour ozone whose values are approaching or are currently exceeding the 8-hour ozone standard, then they may wish to opt-in to the EAC in lieu of the possibility of being declared an 8-hour nonattainment area in 2004. There are several significant impacts from being declared an ozone nonattainment area:

> Transportation conformity budgets must be met or highway funds may be cut off;

- Major new or modified construction in the nonattainment area must offset its emissions to build in the area; and

- The area's economic growth is restricted.

There are several steps in the EAC:

<u>Step#1: The Compact</u>

- Details how the EAC Plan will be developed;

- Lays out enforceable milestones/terms with specific deadlines that must be met or 8-hour ozone planning reverts back to traditional nonattainment area designation approach; and

- Must be signed and submitted to EPA by December 31, 2002.

<u>Step#2: EAC Plan Development</u>

- Component of the EAC Plan include:
  - Emissions Inventory
  - Modeling
  - Control Strategy that Demonstrates Attainment by 2007
  - Maintenance for Growth Planning

- The EAC Plan to be included in a SIP that must be submitted to EPA by December 31, 2004;

- Any adopted rules must be implemented by December 31, 2004 (target is attainment of the 8-hour ozone standard by 2007 relying on three years of monitored ozone data from 2005-2007); and

- Must address emissions growth until at least 2012.

EPA's commitment and safeguards for the EAC are as follows:

- If the area is meeting its EAC milestones/terms at the time of 8-hour ozone nonattainment designations and is violating the 8-hour ozone standard:
  - Effective date of attainment designation and/or designation requirements is deferred.

- If the area attains the 8-hour ozone standard in 2007:
  - The area is redesignated as attainment and there are no further requirements.

- If the area fails to meet the terms and/or milestones of the EAC then:

- The area forfeits participation in the EAC.
- The area enters into the traditional 8-hour ozone implementation process.
- There are no delays or favorable treatment.

> If the area fails to attain the 8-hour ozone standard in 2007 (i.e., violates the 8-hour ozone standard based on 2005-2007 observed air quality data)
>
> - The Area is immediately designated as an 8-hour ozone nonattainment.
> - SIP revision due from State by December 31, 2008.
> - No delay in attainment date.

The timeline for the EAC may undergo revisions and refinement. Based on our current understanding, Table 1-1 summarizes the key dates for the EAC that would likely be incorporated until the EAC Milestones.

**Table 1-1**. Draft key dates for the Early Action Compact (EAC) requirements.

| Date | Item |
|---|---|
| December 31, 2002 | Submit signed EAC with Milestones |
| June 16, 2003 | Identify/describe local strategies being considered for use in the EAC Plan |
| March 31, 2004 | Submit attainment demonstration modeling and The Plan to State |
| December 31, 2004 | State submits SIP with the local Area Plan to EPA |
| December 31, 2005 | Implement any required rules |
| December 31, 2007 | Attain the 8-hour ozone standard |

To meet the technical milestones required by EPA of EAC Protocol participants, the 8-hr ozone modeling and analysis work must be completed by February 2004. Completion on this date will allow the Early Action Compact to proceed through a public comment period and a Colorado Air Quality Control Commission (AQCC) hearing. The final Early Action Compact must also go through a legislative process for submittal to the Environmental Protection Agency-Region VIII. Accordingly, the base year and base projected year (2007) photochemical modeling effort will need to be completed by the end of September 2003. This date will allow the RAQC, CDPHE and other stakeholders the time needed to develop local controls if required. Final attainment year control case modeled demonstrations are needed by December 31, 2003. Consistent with recommendations by the Colorado Air Quality Control Commission, the RAQC has established a stakeholder process including the formation of a modeling subcommittee to guide the ENVIRON/Alpine modeling analyses. Note that EPA has not designated any regions as nonattainment for the 8-hour ozone standard so no formal requirement exists for an 8-hour ozone attainment demonstration.

## 1.2 Elements of the Denver EAC Study

The goal of the Denver EAC 8-hr Ozone Study is to conduct a comprehensive photochemical modeling study for the Denver-Northern Front Range Region (DNFRR) that can be used as the technical basis for 8-hr ozone SIP development. The modeling study, guided by this protocol, is specifically designed to identify the processes responsible for 8-hr ozone exceedances in the region and to develop realistic emissions reduction strategies for their control.

### 1.2.1 Study Objectives

Specific objectives of the Denver EAC study include:

- Prepare an Ozone Modeling Protocol, consistent with EPA requirements, that provides direction to the 8-hr ozone modeling of the Denver-Northern Front Range (this document);

- Collaborate with the CDPHE in the identification and justification of one or more 8-hr ozone modeling episodes for the Denver study (Section 3.0);

- Develop suitable, internally consistent emissions, meteorological and photochemical modeling domains (Section 4.0);

- Construct dynamically and thermodynamically consistent meteorological inputs at appropriate grid scales for direct input to the emissions and photochemical models;

- Process the county-wide base year emissions inventories developed by CDPHE, taking into account appropriate temporal, spatial, and chemical speciation factors as well as adjusting the mobile source emissions to the specific pressure and temperature conditions of the modeling episode(s);

- Produce the model-ready base-year inventories and perform additional quality assurance (QA) of the emissions data sets beyond that conducted by the CDPHE;

- Develop photochemical model base case modeling inputs for the selected modeling episode(s) and carry out base case model performance testing, diagnostic analysis, and pertinent sensitivity studies, including a check on mass consistency;

- Evaluate the photochemical model's performance for the selected episode(s) and compare the results with EPA's performance objectives (EPA, 1991; 1999) for ozone modeling;

- Perform pertinent diagnostic and investigative photochemical model sensitivity tests to better understand model performance, obtain more confidence that the model is working correctly, and obtain a preliminary estimate of ozone source-receptor relationships in the Denver region;

- Develop model-ready year 2007 emissions files from emissions inventories provided by CDPHE and then perform future-year photochemical modeling to assess the likelihood of attainment of the 8-hour ozone NAAQS;

> Perform across-the-board VOC and NOx emissions reduction sensitivity simulations to explore the ozone response for the modeling episode(s);

> Perform additional future-year (2007 or 2012) control scenario simulations to estimate ozone levels in the Denver region under different local control regimes (if the future year baseline modeling does not show attainment with the 8-hr NAAQS);

> Develop suitable "weight of evidence" analyses supporting the ozone attainment demonstration, consistent with EPA guidance;

> Assist the RAQC and CDPHE in developing the technical information to support the documentation required for the Denver 8-hr ozone Early Action Compact protocol;

> Provide for a thorough and efficient transfer of modeling codes, data sets, and related information to other stakeholders in the process including the EPA Region VIII and the CDPHE;

> Participate in mid-project and final project review meetings in Denver; and

> Set up the full suite of models and databases developed in this study on CDPHE computers and provide on-site training in the use of the modeling system(s).

These objectives will be met the following technical approach to be implemented as set forth in this protocol document.

### 1.2.2 Modeling Protocol

This protocol documents the modeling assumptions and activities associated with the Denver EAC 8-hr ozone study. Specific activities discussed in subsequent chapters include: (a) selection of appropriate models, data bases, and episodes, (b) evaluating the performance of the full modeling system, and (c) use of the models and input data bases to estimate the levels of VOC and/or NOx emissions controls potentially needed to maintain and/or attain the 8-hr ozone standard in the DNFRR. The modeling approach identified in this protocol will undergo review by the RAQC, the CDPHE, a modeling subcommittee, other stakeholders, and the U.S. EPA Region VIII. From time to time it may be appropriate to modify the procedures set forth herein as new information becomes available. Major modifications to the study approach will be reviewed with the DEP and the TAG prior to their implementation.

### 1.2.3 Episode Selection

The procedures culminating in the selection of suitable 8-hr ozone modeling episodes are described in detail in the recent report by the CDPHE entitled "Episode Selection for the Denver Early Action Compact". This study by CDPHE staff identified and prioritized five (5) multiple day 8-hr ozone episodes based on a detailed review of the regional air quality and meteorology. This work served as the foundation for subsequent episode selection efforts performed jointly by the CDPHE and the ENVIRON/Alpine team that is discussed in Section 3.0. The result of this process was the selection of the 'summer '02 Episode. Spanning the period 2 June to 22 July 2002, this period encompassed the top three ozone episodes identified in the CDPHE episode selection report.

### 1.2.4 Model Selection

The photochemical modeling system selected for the Denver EAC study consists of three state-of-science regional emissions, meteorological, and nested photochemical air quality simulations models. These include:

> **Emissions Model** -- The EPS2x, recently developed by ENVIRON as an enhanced version of EPA's EPS2.0 modeling system, has been thoroughly tested, used in many SIP regulatory applications, and is more computationally efficient than many existing modeling systems.

> **Meteorological Model** The PSU/NCAR MM5 prognostic meteorological model is the most commonly used model for providing meteorological inputs to emissions and photochemical models for SIP regulatory applications.

> **Photochemical Model** While EPA does not recommend a specific model for regulatory 8-hr ozone modeling, the 8-hr modeling guidelines identifies several state-of-science models that might be considered on a case-by-case basis. The CAMx model was selected for this study because it is publicly available, is computationally efficient, has been peer-reviewed and extensively tested in numerous recent modeling studies, and has a number of new technical improvements of potential benefit to the DNFRR application.

### 1.2.5 Model Evaluation

The MM5 and CAMx models will be evaluated in accordance with EPA guidelines (EPA, 1991; 1999) and procedures currently recommended in the technical community (Tesche et al., 1991; Roth, Tesche and Reynolds, 1998; Seaman, 2000; Russell and Dennis, 2000, Emery et al., 2001). For the entire summer '02 episode, routine surface ozone monitoring and limited NOx data are available. Should speciated volatile organic compound (VOC) data be available, this information will also be used in the performance evaluation. The MM5 model will be evaluated at various spatial scales using available hourly surface and twice daily aloft meteorological measurements. The input and output data sets for all three models will be quality-assured using existing statistical and graphical QA procedures.

### 1.2.6 Future Year Control Strategy Modeling

Assuming satisfactory operation of the meteorological and photochemical modeling systems is demonstrated through performance evaluation exercises, the CAMx model will be used to project 8-hr ozone air quality in the DNFRR in the appropriate future year (e.g., 2007). Should modeled exceedances occur, various anthropogenic emissions reduction strategies will be developed in an attempt to determine the levels of VOC and/or NOx controls needed to attain and/or maintain the 8-hr standard. These control strategies will be formulated through technical discussions with the RAQC and the modeling subcommittee.

### 1.2.7 Schedule, Deliverables, and Reporting

The current schedule for the Denver EAC Study (Figure 1-1) identifies the main project activities including protocol preparation, database development, model evaluation, control scenario development and testing, reporting, and project meetings. Two (2) project meetings are tentatively scheduled although the exact number may change depending upon the specific needs of study. The study is estimated to be completed by 31 March 2004.

The deliverables associated with this study and their estimation submission dates are as follows:

> "Air Quality Modeling Analysis for the Denver Early Action Ozone Compact: Modeling Protocol, Episode Selection, and Domain Definition", 15 May 2003;

> "Air Quality Modeling Analysis for the Denver Early Action Ozone Compact: Meteorological Model Evaluation Report", 31 May 2003;

> "Air Quality Modeling Analysis for the Denver Early Action Ozone Compact: Base Year Photochemical Model Performance Evaluation", 31 August 2003

> "Air Quality Modeling Analysis for the Denver Early Action Ozone Compact: Future Year Baseline Modeling Report", 30 September 2003;

> "Air Quality Modeling Analysis for the Denver Early Action Ozone Compact: Control Scenario Photochemical Modeling Report", 31 December 2003;

> "Air Quality Modeling Analysis for the Denver Early Action Ozone Compact: Draft Technical Support Document", 1 February 2004;

> "Air Quality Modeling Analysis for the Denver Early Action Ozone Compact: Final Technical Support Document", 15 February 2004;

In addition, electronic versions of the model input and output data sets developed in this study will be supplied to the RAQC (or CDPHE) on magnetic media at the conclusion of the project.

## 1.3 Study Participants

Current participants in the Denver EAC study are identified in Table 1-2. The study will be directed by Mr. Gerald Dilley of the RAQC. A modeling subcommittee consisting of representatives from federal and local governments, industry, academia, and public interest groups is being developed and will provide technical expertise and valuable input to the study. The RAQC, aided by technical input from the CDPHE and the modeling subcommittee, will guide the work activities of the contractors (ENVIRON and Alpine Geophysics). This will include, but not be limited to the activities associated with protocol development, episode selection, data base development, model selection and adaptation, model performance evaluation, future year emissions forecasting, control strategy development and testing, formal attainment demonstration efforts, and project reporting.

Specific data analysis, modeling, and reporting activities will be performed by staff at ENVIRON and Alpine Geophysics. Mr. Ralph Morris of ENVIRON will serve as Project Manager. Mr. Morris and Mr. Dennis McNally (Alpine) and will serve as Co-Principal Investigators and participate in all technical aspects of the study. The Co-PI's will also be the primary contractor representatives at project meetings.

### 1.4 Communications

Project communications will be accomplished by occasional technical review meetings in Denver, biweekly telephone conference calls, and *ad hoc* but regular telephone calls and e-mail messages. Where technical difficulties or issues necessitating RAQC assistance arise, they will be brought to the attention of the Denver EAC Protocol (DEP) Project Manager (Mr. Gerald Dilley) via e-mail, by telephone, or if less pressing, through written correspondence. All major issues or concerns will be documented including the nature of the difficulty and the resolution reached between the contractor and the RAQC.

**Table 1-2.** Participants in the Denver EAC 8-Hr Ozone study.

| Organization | Individual(s) | Address | Contact Numbers |
|---|---|---|---|
| ***U.S. EPA*** | | | |
| | Mr. Kevin Golden | Regional Meteorologist<br>EPA Region VIII<br>Denver, CO | bus: (303) 312-6442<br>fax: (303) 312-6064<br>e-mail: golden.Kevin@epa.gov |
| ***Regional Air Quality Council*** | | | |
| | Mr. Kenneth Lloyd | Executive Director<br>1445 Market Street, Suite 260<br>Denver, CO 80202 | bus: (303) 629-5450<br>fax: (303) 629-5822<br>e-mail: klloyd@raqc.org |
| | Mr. Gerald Dilley | Technical Program Manager<br>1445 Market Street, Suite 260<br>Denver, CO 80202 | bus: (303) 629-5450, ext. 240<br>fax: (303) 629-5822<br>e-mail: jdilley@raqc.org |
| ***Colorado Department of Public Health and Environment*** | | | |
| | Ms. Sheila Burns | Air Pollution Control Division<br>4300 Cherry Creek Dr. South<br>Denver, CO 80222 | bus: (303) 692-3223<br>fax: (303) 782-5493<br>e-mail: Sheila.Burns@state.co.us |
| | Ms. Barbara MaCrae | Air Pollution Control Division<br>4300 Cherry Creek Dr. South<br>Denver, CO 80222 | bus: (303) 692-3136<br>fax: (303) 782-5493<br>e-mail:<br>Barbara.Macrae@state.co.us |
| | Mr. Kevin Briggs | Air Pollution Control Division<br>4300 Cherry Creek Dr. South<br>Denver, CO 80222 | bus: (303) 692-3222<br>fax: (303) 782-5493<br>e-mail: Kevin.Briggs@state.co.us |
| ***Colorado Department of Transportation*** | | | |
| | Ms. Lizzie Kemp | 1325 S. Colorado Blvd.<br>Empire Park B606<br>Denver, CO 80222 | bus: (303) 757-9763<br>fax:<br>e-mail:<br>Elizabeth.kemp@dot.state.co.us |
| ***Denver Regional Council of Governments*** | | | |
| | Mr. Eric Sabina | 4500 Cherry Creek Dr. South<br>Suite 800<br>Denver, CO 80246 | bus: (303) 4806789<br>fax: (303) 480-6790<br>e-mail: esabina@drcog.org |
| ***Modeling Subcommittee*** | | | |
| | TBD | | bus:<br>fax:<br>e-mail: |
| ***Contractors*** | | | |
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| Alpine Geophysics | Mr. Dennis McNally<br>Ms. Cyndi F. Loomis | Senior Scientists<br>7341 Poppy Way<br>Arvada, CO 80007 | bus: (303) 421- 4221<br>fax: (303) 421- 9553<br>e-mail:<br>dem@alpinegeophysics.com<br><br>cfl@alpinegeophysics.com |
| Alpine Geophysics | Dr. T. W. Tesche | Principal Scientist<br>3479 Reeves Drive<br>Ft. Wright, KY 41017 | bus: (859) 341-7502<br>fax: (859) 341-7508<br>e-mail: twt@iac.net |

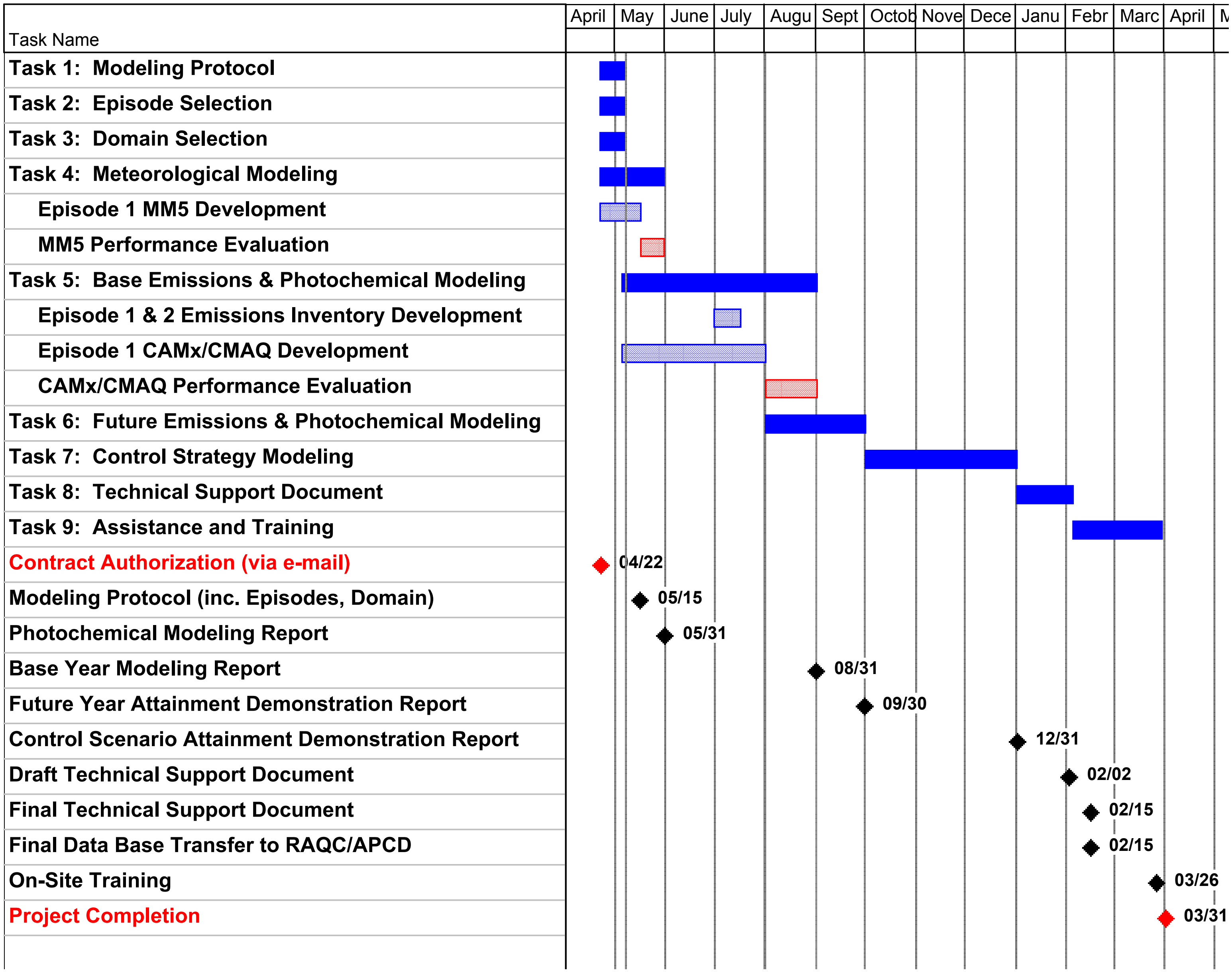



**Figure 1-1.** Schedule for the Denver EAC 8-hr Ozone Modeling study (rev. 15 May 2003).

# 2.0 MODEL SELECTION

This section introduces the models to be used in the Denver 8-hr Early Action Compact ozone study and gives the justification for these selections. The selection methodology presented below follows EPA's draft guidance for regulatory modeling in support of 8-hr ozone attainment demonstrations (EPA, 1999). Unlike the previous guidance for 1-hr ozone modeling (EPA, 1991), the agency now recommends that models be selected on a 'case-by-case' basis with appropriate consideration being given to the candidate model's: (a) technical formulation, capabilities and features, (b) pertinent peer-review and performance evaluation history, (c) public availability, and (d) demonstrated success in similar regulatory applications. All of these considerations should be examined for each class of models to be used (e.g., emissions, meteorological, and photochemical) in part because EPA no longer recommends a specific model or suite of photochemical models for regulatory application.

The models to be used in the Denver EAC study include:

> The Comprehensive Air Quality Model with Extensions (CAMx, Version 4.0) (ENVIRON, 2000);

> The Emissions Processing System (EPS2x) (Mansell and Wilson, 2002) that is an extension of EPS2.0 (EPA, 1992); and

> The PSU/NCAR MM5 Prognostic Meteorological Model (MM5) (Dudhia, 1993; Seaman, 2000).

Below we summarize the main features of these models and then explain why each is an appropriate choice for the Denver study.

## 2.1 Overview of the Recommended Models

### 2.1.1 The Emissions Processing System (EPS2x)

Over the last decade, the need for consistent high quality emissions inventories for regulatory ozone modeling has grown rapidly (Russell and Dennis, 2000). To meet this need, three state-of-science emissions modeling systems have been developed within the past several years: EPS2x, EMS-95 (Wilkinson et al., 1994; AG, 1995) and SMOKE (Coats, 1995). EPS2x (Mansell and Wilson, 2002) is an extension of the earlier EPS2.0 model originally developed by the EPA to support application of the regulatory guideline UAM-IV model (EPA, 1992). EPS2x includes several enhancements to EPS2.0 to treat regional emissions modeling and interface with more recent emission estimates (e.g., MOBILE6). EMS-95 was developed to support the SARMAP and LMOS air quality modeling studies in the early 1990s and was later used in the OTAG, SAMI, and EPA NOx SIP Call modeling programs. The EMS-95 framework formed the basis for the original emissions modeling processor developed for the Models-3/CMAQ system (Byun and Ching, 1999). SMOKE was first applied for regulatory air quality modeling in support of the North Carolina ozone SIP in 1997 and is now installed as the default emissions processing system for the current version of the EPA Models-3 system. These three emissions modeling systems constitute significant scientific and computational advancements beyond EPA's urban-scale (EPS2.0) and regional (FREDS) emissions processing systems originally developed in the mid- to late-1980s (Modica et al., 1985; SAI, 1990).

EPS2x produces temporally and spatially resolved base case and future year area source, stationary source, on-road and non-road mobile source, and biogenic emissions estimates suitable for input to current state-of-science air quality models. The model accommodates the input data requirements of a wide range of contemporary regional photochemical models including CAMx, UAM-V, URM, and Models-3/CMAQ. EPS2x provides reporting and quality assurance functions, a capability that will be important when developing verifying the new modeling emissions databases developed for the Denver study by the CDPHE. EPS2x is designed to identify and handle errant data entries, and has a number of ad-hoc reporting capabilities. EPS2x not only handles the gas phase pollutants but also treats aerosols. Finally, EPS2x can prepare air quality model ready emissions estimates for use with not only CB-IV and SAPRC chemistries but also any chemical mechanism provided the appropriate data are available. Table 2-1 summarizes the current features of the EPS2x.

### 2.1.2 The MM5 Meteorological Model

Historically, there have been several options for developing meteorological fields for ozone SIP model applications – wind interpolation schemes, diagnostic wind models, hybrid interpolation schemes and a few primitive equation models. However, today there are essentially only two state-of-science meteorological models that are recognized for *regulatory applications* of photochemical models (Seaman, 2000). The two most commonly used state-of-science prognostic models for use in urban and regional ozone attainment demonstrations are the public domain Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR) Mesoscale Meteorological Model (MM5) and the Regional Atmospheric Modeling System (RAMS), a proprietary model developed at Colorado State University. Scientific review papers by Pielke and Uliasz (1998) and Seaman (2000) discuss the full range of contemporary models available for air quality simulations. There is little doubt that the MM5 and RAMS models are the most common and appropriate choices for 1-hr and 8-hr SIP related applications.

The non-hydrostatic MM5 model (Dudhia, 1993; Grell et al., 1994) is a three-dimensional, limited-area, primitive equation, prognostic model which has been used widely in regional air quality model applications (see, for example, Russell and Dennis, 2000; Seaman et al., 1995,1997; Seaman, 2000; Seaman and Stauffer, 1996; Tesche et al., 1998a,b). The basic model has been under continuous development, improvement, testing and open peer-review for more than 20 years (see, for example, Anthes and Warner, 1978; Anthes et al., 1977) and has been used world-wide by hundreds of scientists for a variety of mesoscale studies, including cyclogenesis, polar lows, cold-air damming, coastal fronts, severe thunderstorms, tropical storms, subtropical easterly jets, mesoscale convective complexes, desert mixed layers, urban-scale modeling, air quality studies, frontal weather, lake-effect snows, sea-breezes, orographically induced flows, and operational mesoscale forecasting.

MM5 is based on the prognostic equations for three-dimensional wind components (u, v, and w), temperature (T), water vapor mixing ratio ($q_v$), and the perturbation pressure (p'). Use of a constant reference-state pressure increases the accuracy of the calculations in the vicinity of steep terrain. The model uses an efficient semi-implicit temporal integration scheme and has a nested-grid capability that can use up to ten different domains of arbitrary horizontal and vertical resolution. The interfaces of the nested grids can be either one-way or two-way interactive.

MM5 uses a terrain-following non-dimensionalized pressure, or "sigma-p", vertical coordinate similar to that used in many operational and research models. In the non-hydrostatic MM5 (Dudhia, 1993), the sigma levels are defined according to the initial hydrostatically-balanced reference state so that the sigma levels are also time-invariant. The gridded meteorological fields produced by MM5 are directly compatible with the input requirements of air-quality models using this coordinate, such as Models-3/CMAQ. The fields can be used in other regional air quality models with different coordinate systems (e.g., CAMx, URM, UAM-V, and MAQSIP) by performing a vertical interpolation, followed by a mass-conservation re-adjustment (McNally, 1997).

Distinct planetary boundary layer (PBL) parameterizations are available for air-quality applications, both of which represent sub-grid-scale turbulent fluxes of heat, moisture and momentum. These parameterizations each have a surface energy budget equation to predict the ground temperature ($T_g$), based on the insolation, atmospheric path length, water vapor, cloud cover and longwave radiation. The surface physical properties of albedo, roughness length, moisture availability, emissivity and thermal inertia are defined as functions of land-use for 14 categories via a look-up table. One scheme uses a first-order eddy diffusivity formulation for stable and neutral environments and a modified first-order scheme for unstable regimes. The other uses a prognostic equation for the second-order turbulent kinetic energy, while diagnosing the other key boundary layer terms.

Initial and lateral boundary conditions are specified from mesoscale three-dimensional analyses performed at 12-hour intervals on the outermost grid mesh selected by the user. Additional surface fields are analyzed at three-hour intervals. A Cressman-based technique is used to analyze standard surface and radiosonde observations, using the National Center for Environmental Prediction (NCEP) Eta analysis as a first guess. The lateral boundary data are introduced into MM5 using a relaxation technique applied in the outermost five rows and columns of the most coarse grid domain.

A major feature of the MM5 is its use of state-of-science methods for Four Dimensional Data Assimilation (FDDA). The theory underlying this approach and details on how it has been applied in a variety of applications throughout the country are described in depth elsewhere (Seaman et al., 1992, 1995, 1996, 1997; Tesche and McNally, 1996a,b, 1997a-c). All of the meteorological transport fields required to exercise the EPS2x emissions and CAMx photochemical models for the Denver 8-hr modeling episode(s) (e.g., three-dimensional winds, temperatures, PBL heights, diffusivities, cloud fields, and related inputs) will be derived from the MM5 outputs. Table 2-2 summarized the key attributes of the PSU/NCAR MM5 model.

### 2.1.3 The CAMx Regional Photochemical Model

Each of the Eulerian regional photochemical dispersion models identified in EPA's 8-hr modeling guidance were specifically considered for use in the Denver EAC study. As part of the model selection process, we performed a thorough comparison of these models and their suitability for the intended Denver application. From this review, it was determined that the CAMx regional model was most appropriate for the Denver study.

The Comprehensive Air-quality Model with extensions (CAMx) is an established regional photochemical model containing many advanced features such as grid nesting, sub-grid-scale Plume-in-Grid, alternative numerical advection solvers, and a chemical mechanism compiler for rapidly updating the alternative kinetic mechanisms (SAPRC, CBM-IV) in the model (ENVIRON, 1997; 2002; 2003). A significant scientific advancement over the UAM-V, CAMx includes detailed ozone source apportionment technology (OSAT), process analysis (PA), and the Decoupled Direct Method (DDM) sensitivity analysis algorithms (ENVIRON, 2002; 2003; Dunker et al., 2002a,b). Due to it's public availability and inclusion of many new science features (e.g., source apportionment, process analysis, flexible chemical mechanism compiler, alternative numerical advection schemes and chemical kinetic mechanisms), CAMx is being (or has been) used widely in support of 1-hr and 8-hr SIP modeling studies throughout the U.S. (e.g., Houston/Galveston, Beaumont/Pt. Arthur, Pittsburgh, Cincinnati-Hamilton, Kansas City/Missouri, Peninsular Florida, and the San Francisco Bay Area). CAMx Version 3.1 (ENVIRON, 2002) is currently available for downloading from the website: www.camx.com. A newer version, CAMx Version 4 that includes aerosol chemistry and other significant modeling advancements will be publicly available in April 2003 (ENVIRON, 2003). For the RAQC Denver EAC 8-hour ozone modeling study we intend to use the latest CAMx Version 4 model. The specific attributes of the CAMx model are summarized in Table 2-3.

## 2.2 Justification for Model Selection

### 2.2.1 EPS2x

The EPS2x is recommended as the emissions model for the Denver EAC study for the following reasons:

> EPS2x is a mature, thoroughly-tested emissions modeling system having been employed by a wide variety of users governmental, commercial, academic, and private users in numerous regions throughout the U.S. and abroad;

> ENVIRON/Alpine staff have considerable experience with the model, in part because ENVIRON staff members participated heavily in the original design and coding of the model and in many of the subsequent refinements and model extensions;

> All of the regional emissions data sets developed by the CDPHE for the Denver study can be easily processed and QA'd using EPS2x. The emissions data

processed by EPS2x can be directly incorporated into the nested 12/4/1.33 km CAMx modeling grids to be used in this study (see section 4);

> The EPS2x provides several quality assurance and error checking routines, thereby allowing the study team to perform an independent verification of the base year and future year emissions inventories developed for this project by the CDPHE; and

> Many of the future year emissions controls likely to be examined in Denver EAC are similar to those considered in developing 1-hr and 8-hr control scenarios in other recent SIP applications (e.g., Pittsburgh-Beaver Valley, Cincinnati-Hamilton, Kansas City-St. Louis, Houston/Galveston, Dallas-Fort Worth, etc.); consequently, time and resources can be saved and potential errors minimized by using the readily available data sets and the EPS2x model.

> EPS2x (and EMS95 for that matter) contains superior quality assurance and quality control (QA/QC) functions to the SMOKE emissions modeling system, which is an important, attribute given the time schedule for the Denver 8-hour EAC modeling requirements.

> EPS2x is written in Fortran whose compilers are routine available on computers used for photochemical modeling, as compared to EMS95 that is based on the SAS software which requires a license and special expertise to operate.

### 2.2.2 MM5

Currently, the two most commonly used state-of-science prognostic meteorological models to support air quality modeling are the MM5 and the Regional Atmospheric Modeling System (RAMS). A number of recent studies inter-compare the theoretical formulations and operational features of these models (see, for example, Mass and Kuo, 1998; Seaman, 1995, 1996; Pielke and Pearce, 1994) and evaluate their performance capabilities under a range of atmospheric conditions (e.g., Cox et al., 1998; Hanna et. al., 1998; Seaman et al., 1992, 1995, 1996; Tesche and McNally, 1993a-f; McNally and Tesche, 1996a,b,f; 1998c). There have also been a number of studies involving ‘side-by-side’ comparative performance evaluations of MM5 and RAMS for the OTAG and LMOS episodes (Tesche and McNally, 1996b; Tesche et. al., 1997a; Tesche et al., 1999a).

The MM5 is recommended as the prognostic meteorological modeling component for the Denver study for the following reasons:

> All of the available state-of-science regional photochemical models identified in EPA’s 8-hr modeling guidance can be operated without difficulty using inputs supplied by the MM5; however, some ozone models such as MAQSIP and Models-3/CMAQ cannot be run easily with the RAMS polar stereographic map projection. In some cases, costly software development would be needed to allow this coupling between RAMS and certain air quality models;

- In a recent scientific model inter-comparison (Tesche et al., 2003) examining nearly fifty air quality applications across the country, the MM5 model was found to perform somewhat better than RAMS, particularly for surface and aloft winds and surface temperatures;

- The MM5 model has a far richer application history in regulatory ozone modeling studies compared with RAMS. While RAM's principal air quality applications have been in OTAG and SAMI, the MM5 has been employed in a much wider range of regional studies including OTAG, SAMI, NARSTO, SARMAP, SCOS, SCAQS as well as in a number of urban-scale SIP applications (e.g., Pittsburgh, Cincinnati, Denver, Kansas City, St. Louis);

- The MM5 has been applied successfully to the Denver Front Range Region as part of the Denver Air Quality Study (see, for example, McNally and Tesche, 1997d; 1998);

- While ENVIRON/Alpine have extensive experience exercising both MM5 and RAMS in different urban and regional-scale studies, in most regulatory ozone applications the MM5 model has been the preferred system; and

- Finally, EPA's draft 8-hr modeling guidance disallows (or at least discourages) the use of proprietary models. The RAMS model has required the purchase of licenses in the past so has been considered proprietary. More recently the RAMS developers are making the model available without fees for governmental applications, any stakeholder application would still be subjected to the license fees. With MM5 being publicly available with no restriction on its use, this fact alone strongly supports selection of MM5.

### 2.2.3 CAMx

During the recent 1998 NARSTO Critical Tropospheric Ozone Assessment, two major reviews of photochemical modeling were performed. First, Russell and Dennis (2000) compared the scientific and operational features of essentially all current recent Eulerian photochemical models in use up to that time. Second, Roth, Tesche and Reynolds (1997) reviewed more than twenty regulatory applications of photochemical models in the U.S. and Canada. From these reviews and the study team's own experience with each of these models, we recommend CAMx as the principal ozone modeling tool for the Denver EAC study. Conceivably, other models (e.g., CMAQ), might also be utilized in supporting roles (e.g., model diagnosis, sensitivity analysis, weight of evidence, corroboration) if appropriate. CAMx is recommended as the photochemical model for Denver EAC study for the following reasons:

- CAMx is a more scientifically advanced model than the urban UAM-IV model that has been EPA's preferred ozone guideline model in the past (Russell and Dennis, 2000; Tesche et al., 1992);

> CAMx has undergone extensive successful testing by a variety of groups using the 1991 and 1995 OTAG databases (see, for example, Lurmann and Kumar, 1997; McNally and Tesche, 1998a, McNally et al., 1998a-c; Tesche and McNally, 1998a; Tesche et al., 1998c,e,f);

> CAMx is unique among state-of-science air quality models in its ability to offer ozone source apportionment technology (OSAT), process analysis, and the DDM sensitivity analysis scheme; and

> CAMx is a public-domain model, available free of charge, without restriction, and without a mandatory 'waiting period'. It is available to all interested users.

## 2.3 Summary of Model Selection and Justification

In summary, we recommend the EPS2x, MM5 and CAMx regional models for use in the Denver EAC study. In this chapter, we have introduced the models in the context of the current state-of-science in emissions, meteorological, and photochemical modeling and have provided brief technical summaries of each one. In addition, we have presented the rationale underpinning the selection of this specific suite of models for the Denver study.

We conclude the model selection discussion by presenting in Tables 2-4 through 2-6 the six (6) criteria set forth in EPA's draft 8-hr modeling guidance for determining whether a candidate model is ***appropriate*** for use in an ozone attainment demonstration study. Associated with each of the six criteria are the reasons why we believe the three models are indeed suitable candidates for this application. Tables 2-7 through 2-9 list the five (5) criteria that EPA has established for actually ***justifying*** the use of a model in the proposed study. Collectively, the information presented in Tables 2-4 though 2-9 supports the contention that the EPS2x, MM5 and CAMx are logical choices given the specific technical, regulatory, and resource aspects of the Denver Early Action Compact study.

**Table 2-1.** Attributes of the EPS2x emissions modeling system.

| Model Attribute | EPS2x |
|---|---|
| Model Name | Emissions Processing System (EPS2x) |
| Developer | EPA and ENVIRON International Corporation<br>EPA (1992), (Mansell and Wilson, 2002) |
| Availability | Free, public-domain model |
| Degree of Development | Mature modeling system; significant peer-review and broad experience in application studies |
| Input Requirements | Land use/land cover information, area source emissions by category, VMT and link data; point source facility data and annual emissions rates. |
| Gas-Phase Pollutants Treated | CO, NOx, VOC |
| Particulate Pollutants Treated | Size fractionated, chemically speciated primary particulate emissions |
| Computer Platform | SUN, DEC, SGI and IBM Unix workstations, Linux workstations. |
| Software Requirements | Fortran |
| Examples of Inventory Development Studies in Support of Air Quality Modeling Studies | Houston/Galveston 1-Hour Ozone SIP (TCEQ, 2002), Dallas-Fort Worth 1-Hour Ozone SIP (TCEQ, 1999), East Texas EAC Analysis (ENVIRON, 2002). Oklahoma EAC Study (ENVIRON, 2002). |
| Peer Review | EPA |
| Documentation | Complete user documentation in Mansell and Wilson (2002) and EPA (1992) |
| Noted Strengths | Facilitates quality assurance (QA), error checking, and reporting functions;<br>Integrates with current state-of-science photochemical/PM models;<br>Extensive application history by numerous groups in many urban and regional domains<br>Extended to treat regional inventories computationally efficiently |
| Noted Limitations | Extended computational time for domains with many grid cells |
| Equations and Processing | Traditional processing using FORTRAN 77 programming language |
| Coordinate System | Lambert Conformal, Polar Stereographic, Geographic,<br>State plane, Albers equal area, or UTM (Mercator) |
| Spatial Resolution<br>-Horizontal<br>-Vertical<br><br>- Nesting | <br>Variable (1 to 36 km typically) for finite difference and finite element schemes<br>Point source input file, plume rise calculated outside of EPS using postprocessor if necessary<br>Multiple nests and multi-scale nests available |
| Spatial Allocation Capability | Allows flexible user-defined grid domains, spatial resolution and data overlays |
| Model Output | Generates CB-IV, RADM2, and SAPRC outputs for UAM-IV, UAM-V, CAMx, CALGRID, MAQSIP,UAM-AERO, SAQM, SAQM-AERO, and Models-3/CMAQ models |
| Mobile Source Treatment | Mobile 5b, Mobile 6, EMFAC (California model)<br>Link-based interface module available |
| Biogenics Treatment | GLOBEIS, BEIS-2, BEIS-3 |
| Output File Formats | UAM binary format or ASCII |

**Table 2-2.** Attributes of the PSU/NCAR MM5 prognostic meteorological model.

| Model Attribute | MM5 |
|---|---|
| Model Name | Mesoscale Meteorological Model, (Version 5) |
| Developer | Pennsylvania State University, National Center for Atmospheric Research<br>Dudhia (1993); Grell, Dudhia and Stauffer (1994) |
| Availability | Free, public-domain model |
| Forecast Variables | Three dimensional wind components, temperature, water vapor, cloud water/ice, rain water/ice, and the perturbation pressure. |
| Input Requirements | 3-hourly surface data and 12-hourly soundings plus gridded pressure level data set (horizontal winds, temp., R.H. as a function of pressure) for model initialization, BC's and FDDA. Also requires topography, sea-surface temp., and land use. |
| Computer Platforms | Most popular workstations (e.g., SUN SPARCstation, IBM RISC); PC's running LINUX, including clusters. |
| Hardware Requirements | RAM = ~512 MB; Free hard disk = 100Gb; |
| Software Requirements | UNIX, FORTRAN 77, NCAR Graphics |
| Evaluation Studies for Air Quality Model Applications | ***Gulf Coast:*** Tesche and McNally (1998c); Douglas et al, (1999)<br>***NARSTO-NE***: Seaman and Michelson (1998); Tesche and McNally (1996b,f); McNally and Tesche 1996d); Zhang and Rao (1999)<br>***RADM***: Dennis et al., (1990)<br>***OTAG***: McNally and Tesche (1996a,b);Tesche and McNally (1996b,d)<br>***SARMAP***: Seaman, Stauffer, and Lario (1995); Seaman and Stauffer (1996); Tesche and McNally (1993e,f); Tanrikulu (1999); Tesche et al., (1998b)<br>***LMOS***: Shafran and Seaman (1998); Tesche and McNally (1999c)<br>***Los Angeles:*** Seaman et al. (1996, 1997); Tesche and McNally (1997c); Pai et al. (1998); Steyn and McKendry (1988); Tesche et al., (1997e)<br>***Denver Front Range:*** McNally and Tesche (1998c)<br>***Florida:*** Green et al. (1998)<br>***Texas Gulf Coast:*** Emery et al., (2001); TCEQ (2002); McNally and Tesche (2002)<br>***Cincinnati-Hamilton SIP***: Tesche and McNally (1998e)<br>***Pittsburgh-Beaver Valley SIP:*** McNally and Tesche (1996c)<br>***Kansas City/St. Louis SIP:*** Emery et al., (1999);McNally and Tesche (1999c). |
| Peer Review | Pielke (1984); Barchet and Dennis (1990); Tesche and McNally (1993e,f); Pielke and Pierce (1994); Seaman (1995, 2000) |
| Documentation | 5-Volume User's Manuals (Gill, 1992); Twice-annual tutorial classes for new outside users; on-line consultant helpline (NCAR). |
| Noted Strengths | Supports multi-scale FDDA for both analysis and special asynoptic data; turbulent exchange based on TKE; selection of advanced convective parameterizations. |
| Noted Limitations | Extended computational time, particularly for smaller (i.e., 4 km or less) grid scales |
| Equations | Primitive equation model, Non-hydrostatic (non-hydrostatic option) |
| Grid Differencing Scheme | Arakawa-B staggered. |
| Spatial Resolution<br>-Horizontal<br>-Vertical<br>- Nesting | <br>Variable (1 to 200 km)<br>Variable/stretched<br>Multiple/2-way/movable during simulation |
| Coordinate System<br>- Horizontal<br>- Vertical | <br>Mercator; Lambert Conformal; Polar Stereographic<br>Sigma-p (terrain-following) |
| Nesting Scheme | Multiple, moving, overlapping nesting with two-way interaction and pre-defined nest ratios of 3:1 |

| Model Attribute | MM5 |
|---|---|
| Initialization | Cressman objective analysis on pressure surfaces (independent data analysis) |
| Numerics<br>- Time differencing<br><br>- Advection | <br>Leapfrog; split semi-implicit time differencing<br><br>$4^{th}$-order leapfrog |
| Boundary Conditions<br>- Top<br><br>- Surface<br><br>- Lateral | <br>Absorbing layer<br><br>Prognostic surface temperature; NCEP/OSU soil-moisture scheme (Seaman, 1998) based on land use.<br><br>Time-dependent and inflow/outflow dependent |
| Parameterizations<br>- Radiation<br><br>- Explicit moist physics<br><br>- Deep convection<br><br>-Surface layer<br><br>- Boundary layer | Shortwave and longwave schemes that interact with the atmosphere, including cloud and precipitation fields as well as with the surface (Dudhia, 1989).<br><br>Liquid, ice, and mixed phase<br><br>Large-scale processes treated explicitly.  Various convective precipitation modules available including Kuo (1974), Kain-Fritsch (1990, 1993), Fritsch-Chappell, Betts-Miller, modified Arakawa-Schubert (1974), Grell et al., (1991), and Anthes-Kuo (Anthes, 1977).<br><br>Heat, momentum, and water vapor fluxes (Blackadar; Gayno-Seaman)<br><br>Simple bulk aerodynamic parameterization (Blackadar), revised non-local Blackadar (Zhang and Anthes, 1982), Level-2.5 Mellor-Yamada (1974, 1982), or 1.5-order turbulent kinetic energy (TKE) scheme (Gayno et al., 1994). |
| FDDA Capability | Multi-scale, both analysis-nudging and observation-nudging, data use sensitive to orography, 3-D weighting functions<br><br>Nudged parameters: *u,v* winds, temperature, water vapor mixing ratio. |

**Table 2-3.** Attributes of the CAMx regional photochemical model.

| Model Attribute | CAMx |
|---|---|
| Model Name | Comprehensive Air Quality Model with Extensions CAMx (Version 4.0) |
| Developer | ENVIRON International Corporation<br>ENVIRON (2000; 2002; 2003) |
| Availability | Free, public-domain model |
| Input Requirements | 18 files: Met (7), Surface Characteristics (1), Emissions (2), IC/BC (3), Chemistry (3), Control (2) |
| Computer Platforms | SUN, DEC, SGI, RISC, Linux/PC |
| Hardware Requirements<br>- Memory<br>- Input Files<br>- Output Files | Depends on application, typical values are:<br>109 Mbytes<br>200 Mbytes per day<br>220 Mbytes per day |
| Software Requirements | UNIX operating system, FORTRAN 77 |
| Examples of Air Quality Model Evaluations and SIP Applications Studies | ***OTAG***: Emigh et al., (1997); McNally and Tesche (1997c;1998b)<br>***LMOS***: McNally, Tesche and Russell (1996); McNally et al., (1996; 1997); Tesche et al., (1999b)<br>***COAST***: Durrenberger et al., (1999a,b)<br>***NARSTO-NE***: McNally and Tesche (1997d); Morris, Tesche and Lurmann (1999); Tesche and McNally (1998a) Morris et al., 2002<br>***Midwestern U.S.*** McNally and Tesche (1999a); McNally et al., (1998a); Tesche and McNally (1998b; 1998g; 1999d); Tesche et al, (1998c,e)<br>***Northeastern U.S.*** Tesche, McNally, and Loomis (1998h); Tesche et al. (1998g,h)<br>***Baltimore/Washington:*** McNally et al., (1998c)<br>***Chicago:*** Tesche et al., (1999a)<br>***Cincinnati:*** Tesche, McNally and Loomis (1998f,g)<br>***Kansas City/St. Louis***: Tesche et al. (1998f)<br>***Pittsburgh:*** McNally et al., (1998b); Tesche et al., (1997d)<br>***Eastern Pennsylvania***: Tesche, McNally and Loomis (1999b)<br>***Virginia:*** Tesche et al., (1998g) |
| Peer Review | Kumar and Lurmann (1997); Russell and Dennis (2000) |
| Documentation | Code, user's guides, and other user's documentation may be downloaded from the ENVIRON website, i.e., **www.camx.com** |
| Noted Strengths | Plume-in-Grid Treatment<br>Variable Two-Way Grid Nesting<br>User-specified Grid Structure<br>Includes Ozone Source Apportionment Technology (Yarwood et al., 1996a,b)<br>Includes Chemical Mechanism Compiler to allow use of user-specified mechanisms<br>Winds and temperature for each time step are interpolated from the hourly values instead of using the same date for the entire hourly time step |
| Noted Limitations | Extended computational time when many grids cells are used |
| Equations | Three-dimensional, time-dependent species continuity equation |
| Spatial Resolution<br>- Horizontal<br>- Vertical | <br>1 to 36km with a 36/12/4km two-way next typically used<br>Non-uniform vertical grid capability |
| Coordinate System<br>- Horizontal<br>- Vertical | <br>Mercator, Lambert Conformal, Polar Stereographic<br>Terrain-following height coordinates |
| Nesting Scheme | Two-way nesting; several levels of nesting can be accommodated |
| Initialization | Model typically initialized two days prior to time period of interest |

| Model Attribute | CAMx |
|---|---|
| Numerics | Bott, (1989), PPM (Cholla and Woodward, 1984) horizontal advection schemes |
| Boundary Conditions<br>- Top<br>- Lateral | <br>User-specified clean air values<br>User-specified clean air values |
| Species Treated as Primary Emissions | Several Classes of ROG (depends on chemical mechanism), SO2, SO4, NO, NO2, CO, NH3 |
| Treatment of Point Sources | Sub-grid scale point source plumes treated with the Greatly Reduced Execution and Simplified Dynamics (GREASD) Plume in Grid (PiG) module; Released into grid cell in layer corresponding to effective plume height |
| Treatment of Area Sources | Uniform over surface grid cell |
| Grid Structure | Cartesian (UTM, Polar Stereographic or Lambert Conformal), Lat/Long |
| Horizontal Resolution | 1- 4 km (urban)<br>12-36 km (regional) |
| Vertical Resolution | User specified, spatially and temporally varying or invariant layers<br>Typically 7 to 12 layers |
| Meteorology | Prognostic model (e.g., MM5, RAMS) |
| Transport | 3-D wind field |
| Vertical Diffusion | Derived from meteorological inputs using MM5CAMx or RAMSCAMx processor using local Richardson number and/or PBL heights |
| Horizontal Diffusion | Function of deformation characteristics of horizontal wind fields (Smagorinsky, 1963) proportional to grid spacing |
| Gas Phase Chemistry | Updated CBM-IV(Yarwood and Burton, 1993; Whitten et al., 1997); flexible mechansim<br>SAPRC99 Chemical Mechanism Option |
| Photolysis Rates | TUV light model adapted from Madronich and Weller (1990)<br>Cloud impacts on photolysis rates using the RADM algorithm |
| Aqueous Phase Chemistry | RADM bulk module |
| Aerosol Treatment | ISSOROPIA equilibrium |
| Cloud Processes | Option 1 is 2-D cloud field with simplified attenuation of photolysis rates<br>Option 2 is 3-D cloud inputs with integrated attenuation or enhancement of photolysis rates |
| Wet Deposition | Simple treatment using scavenging coefficient approach of Maul (1980) as implemented in CALPUFF (EPA, 1995) or more complex mass transfer and particle rainout and washout if aqueous-chemistry is specified |
| Dry Deposition | Deposition velocity approach: function of atmospheric stability, wind speed, land type and species based on Wesley (1989); Improvements based on Kumar et al., (1996) and Louis (1979) |

**Table 2-4.** Factors qualifying EPS2x for consideration as the emissions model for the Denver EAC study.

| Consideration | Qualification |
|---|---|
| **The model has received a scientific peer review.** | A formal scientific review of the original EPS2.0 modeling system was conducted by Tesche (1991b). Since that time numerous governmental and private modeling groups in the U.S. and abroad have reviewed the model code as part of training, model set-up, exercise, and quality assurance activities. |
| **The model can be demonstrated to be applicable to the problem on a theoretical basis.** | The EPS2x modeling system was explicitly designed to treat all categories of anthropogenic and biogenic emissions source in a modeling framework suitable for input to episodic Eulerian photochemical dispersion models. The model provides hourly resolved, gridded, chemically speciatiated, and source category specific emissions estimates for the important known precursors of photochemically produced ozone. EPS2x is one of three state-of-science regional emissions models actively used in the U.S. and abroad. The features and capabilities of the EPS2x modeling system are consistent with the application on a combined urban- and regional-scale, as required in the Denver EAC Study. |
| **Date bases needed to perform the analysis are available and adequate.** | All input data bases to the EPS2x modeling system (e.g., point, area, and motor-vehicle sources plus biogenic sources are readily available from the CDPHE. Additional high-resolution travel-demand motor vehicle emissions data bases are also available from the Denver Regional Council of Governments (DRCOG's). Model inputs will be prepared following EPA guidelines and those of the model developers. The adequacy of the input data bases developed by the CDPHE will be assessed as part of the EPS2x QA process. |
| **Available past appropriate performance evaluations have shown the model is not biased toward underprediction.** | There are very limited data sets with which to verify emissions models. Major point source emissions estimates are commonly based on continuous emissions monitoring (CEM). On road motor vehicle emissions estimates are based on the EPA Mobile 6. |
| **A protocol on methods and procedures to be followed has been established.** | The protocol is outlined in this document. The EPS2x modeling will be performed in a manner that is consistent with established practice and EPA guidelines regarding air quality modeling related to the 8-hr ozone standard. |
| **The developer of the model must be willing to make the source code available to users for free or for a reasonable cost, and the model cannot otherwise be proprietary.** | EPS2x has been in the public domain since it's original development by EPA in the early 1990s. Copies of the source code, user's guide, and test model inputs can be obtained from the model developer. |

**Table 2-5.** Factors qualifying MM5 for consideration as the photochemical model for the Denver EAC study.

| Consideration | Qualification |
|---|---|
| **The model has received a scientific peer review.** | Formal scientific reviews of the MM5 model have been widely carried out in the U.S. and abroad over the past 20 years. Examples include Pielke (1984); Barchet and Dennis (1990); Tesche and McNally (1993e,f); Pielke and Pierce (1994); and Seaman (1995, 2000). More than one hundred governmental, academic, industrial and private modeling groups in the U.S. and abroad have reviewed the model code as part of training, model set-up, exercise, and quality assurance activities. |
| **The model can be demonstrated to be applicable to the problem on a theoretical basis.** | By design, the PSU/NCAR MM5 model explicitly or implicitly represents the various physical and microphysical processes relevant to the prediction of mesoscale atmospheric phenomena. The model has been used world-wide by hundreds of scientists for a variety of mesoscale studies, including cyclogenesis, polar lows, cold-air damming, coastal fronts, severe thunderstorms, tropical storms, subtropical easterly jets, mesoscale convective complexes, desert mixed layers, urban-scale modeling, air quality studies, frontal weather, lake-effect snows, sea-breezes, orographically induced flows, and operational mesoscale forecasting. The features and capabilities of the MM5 modeling system are consistent with the application on a combined urban- and regional-scale, as required in the Denver study. |
| **Date bases needed to perform the analysis are available and adequate.** | The surface and upper air meteorological data required to exercise and evaluate MM5 are available routinely from the National Weather Service. Large-scale data bases needed for model initialization and boundary conditions are available from the National Center for Environmental Prediction (NCEP) and the National Center for Atmospheric Research (NCAR). These data sets include surface and aloft wind speed, wind direction, temperature, moisture, and pressure. Hourly surface data for model evaluation are available from many AClass I@ airports, i.e., larger-volume civil and military airports operating 24-hour per day. The standard set of upper air data are provided by rawinsonde soundings launched by the NWS every 12 hours from numerous sites across the continent. In addition, NOAA/NCAR operate continuous hourly RADAR profiler sites that report upper-air meteorological measurements at approximately 30 sites throughout the central U.S. Model inputs will be prepared following the guidelines recommended by the model developers and the adequacy of the input data bases will be assessed as part of the MM5 model performance evaluation. |
| **Available past appropriate performance evaluations have shown the model is not biased toward underprediction.** | A number of studies have examined the theoretical formulation and operational features of the MM5 model (see, for example, Mass and Kuo, 1998; Seaman, 1995, 1996; Pielke and Pearce, 1994), the performance of the model under a range of atmospheric conditions (e.g., Cox et al., 1998; Hanna et. al., 1998; Seaman et al., 1992, 1995, 1996; Tesche and McNally, 1993a-f; McNally and Tesche, 1996a,b,f; 1998c), and the performance of the model when compared with other models (e.g., RAMS) for various regional modeling episodes including the OTAG and LMOS episodes (Tesche and McNally, 1996b; Tesche et. al., 1997a; Tesche et al., 1999a). No significant, unexplained bias in the model's estimates of state variables has been encountered. MM5 is one of two state-of-science mesoscale prognostic meteorological models actively used in the U.S. and abroad as input to regional photochemical dispersion and emissions models. |
| **A protocol on methods and procedures to be followed has been established.** | The protocol is outlined in this document. The MM5 modeling will be performed in a manner that is consistent with established practice and EPA guidelines regarding air quality modeling related to the 8-hr ozone standard. |
| **The developer of the model must be willing to make the source code available to users for free or for a reasonable cost, and the model cannot otherwise be proprietary.** | MM5 has been in the public domain since it's original development in the early 1980s. Free copies of the source code, user's guide, and test model inputs can be obtained from the National Center for Atmospheric Research, the Pennsylvania State University, and the U.S. EPA Office of Research and Development. Copies of ancillary data sets and model applications and evaluation software are available from various governmental agencies (e.g., the California Air Resources Board), academic institutions, National Laboratories, and consulting firms. |

**Table 2-6.** Factors qualifying CAMx for consideration as the photochemical model for the Denver EAC study.

| Consideration | Qualification |
|---|---|
| **The model has received a scientific peer review.** | Formal scientific reviews of the CAMx model have been widely carried out since the model was first introduced in the mid 1990s. Examples include Kumar and Lurmann (1997); Russell and Dennis (2000); Sonoma Technology (1997a,b); Reynolds and Roth (1997); TNRCC (1998); McNally et al. (1997a,b; 1998); Lehmann (1998); Morris et al., (1998); and Yocke et al., (1996). More than two-dozen governmental, academic, industrial and private modeling groups have reviewed the model code as part of training, model set-up, performance evaluations, regulatory applications, and quality assurance activities. |
| **The model can be demonstrated to be applicable to the problem on a theoretical basis.** | The CAMx modeling system represents either explicitly or implicitly the physical and chemical processes that are currently known to influence the formation and transport of ozone as well as the emissions, chemical transformation, and dispersion of ozone precursor pollutants. The features and capabilities of the CAMx modeling system are consistent with the application on a combined urban- and regional-scale, as required in the Denver EAC study. |
| **Date bases needed to perform the analysis are available and adequate.** | The CAMx modeling system requires several different types of input data including land use, topographic, air quality, meteorological, and demographic. All of these data sets are routinely available from state or federal agencies. Model inputs will be prepared following EPA guidelines and the adequacy of the input data bases will be assessed as part of the CAMx model performance evaluation. |
| **Available past appropriate performance evaluations have shown the model is not biased toward underprediction.** | The CAMx modeling system has undergone extensive third party review and performance testing and many prior evaluations and applications. Examples of recent model performance evaluations include: Sonoma Technology (1997a,b); Reynolds and Roth (1997); TNRCC (1998); McNally et al;., (1997a,b; 1998a,b,c); Lehmann (1998); Morris et al., (1998); Yocke et al., (1996); Emigh et al., (1997); McNally and Tesche (1997c,d;1998b); McNally, Tesche and Russell (1996); McNally et al., (1996; 1997); Durrenberger et al., (1999a,b); Morris, Tesche and Lurmann (1999); Tesche and McNally (1998a,b; 1998g; 1999a,d); Tesche et al, (1998c,g,h,e; 1999a,b,d,f,g); Tesche, McNally and Loomis (1998f,g,h); McNally and Loomis (1999b). Collectively, these evaluation studies do not reveal the presence of significant, unexplained underestimation bias for ground-level ozone concentrations. |
| **A protocol on methods and procedures to be followed has been established.** | The protocol is outlined in this document. The CAMx modeling will be performed in a manner that is consistent with established practice and EPA guidelines regarding air quality modeling related to the 8-hr ozone standard. |
| **The developer of the model must be willing to make the source code available to users for free or for a reasonable cost, and the model cannot otherwise be proprietary.** | CAMx has been in the public domain since it's original development in the mid 1990s. Free copies of the source code, user's guide, and test model inputs can be obtained from the model developer's website at www.camx.com<br>Copies of ancillary data sets and model applications and evaluation software are available not only from the model developer (ENVIRON International) but also from various governmental agencies (e.g., TCEQ), academic institutions, and consulting firms. |

**Table 2-7.** Factors justifying EPS2x as the emissions model for the Denver EAC study.

| Consideration | Rationale for Selection |
|---|---|
| **Nature of air quality problem leading to non-attainment of the ozone NAAQS should first be assessed, and the selected model should have the attributes and capabilities consistent with the perceived nature of the problem.** | EPS2x is designed for the preparation of detailed urban- and regional-scale photochemical modeling inventories such as are required for the Denver EAC study. EPA's BEIS-3 emissions model and ENVIRON's GLoBEIS model are state-of-science models widely recommended for use in estimating biogenic emissions, which are expected to play an important role in ozone formation in the study area. Mobile 6 is the current operational version of EPA's model for on-road mobile sources and is included in the EPS2x system. Use of Mobile6 facilitates the use of county-level estimates of vehicles miles traveled (VMT) and detailed surface temperature. Where feasible, output from the transportation models from local planning organizations (DRCOG's) will be employed. |
| **Availability, documentation and past performance should be satisfactory.** | EPS2x, BEIS-3, GloBEIS, and Mobile6 are publicly available at no charge from the U.S. EPA or ENVIRON. These models have been successfully used in a variety of regional modeling studies including OTAG, SAMI, and the EPA NOx SIP Call. |
| **Relevant experience of available staff and contractors should be consistent with choice of a model.** | The emissions modeling tasks in the Denver EAC study will be performed by ENVIRON staff who were on the original development team of the EPS2.0 model and have continued to play a role in the model's refinement and evaluation for nearly a decade. ENVIRON staff also have extensive experience in the use of the BEIS-3 and Mobile 6 emissions models. |
| **Time and resource constraints may be considered.** | Use of the EPS2x, BEIS-3, GloBEIS, and Mobile6 models is consistent with the Denver EAC project schedule and budget. |
| **Consistency of the model with what was used in adjacent regional applications should be considered.** | EPS2x, BEIS-3, GloBEIS, and Mobile 6 models (or their predecessors) have been applied in several recent photochemical modeling studies including the OTAG modeling, the EPA NOx SIP Call, the EPA Tier II/Sulfur modeling analysis, the SAMI regional modeling study, the Pittsburgh-Beaver Valley SIP, the Cincinnati-Hamilton SIP, and in more than a dozen other regional ozone modeling studies. The system has also been used in 8-hr ozone modeling studies in Texas and Oklahoma. |

**Table 2-8.** Factors justifying MM5 as the meteorological model for the Denver EAC study.

| Consideration | Rationale for Selection |
|---|---|
| **Nature of air quality problem leading to non-attainment of the ozone NAAQS should first be assessed, and the selected model should have the attributes and capabilities consistent with the perceived nature of the problem.** | The MM5 modeling system is expected to allow a physically realistic, dynamically consistent simulation of the mountain-valley circulation regime over the Colorado Front range as well as other mesoscale features including drainage flows, convergence zones, cumulus convection, and so on. The nested grid feature of MM5 will directly support the urban- to regional-scale nesting scheme in CAMx. |
| **Availability, documentation and past performance should be satisfactory.** | The MM5 modeling system is publicly available and has been frequently used in support of EPS2x and CAMx modeling studies in the eastern U.S. MM5 has also been used to support regional-scale modeling of the southeastern U.S. and has been used for several air quality studies in the western U.S. including the SCAQS, SCOS, and SARMAP studies. It has been used in 1-hr ozone attainment demonstrations in the Pittsburgh-Beaver Valley and Cincinnati-Hamilton areas, is now being used for the 8-hr modeling in the Kansas City/Missouri region, and is being used in the GCOS study as well. Versions of the MM5 have been used for the past 20 years in support of a variety of mesoscale research projects. Results of numerous model evaluation studies with the MM5 reveal that the model performs as well or better than any other mesoscale, applications-oriented, public domain model (Seaman, 2000). |
| **Relevant experience of available staff and contractors should be consistent with choice of a model.** | The MM5 modeling will be performed by AG staff who are thoroughly knowledgeable of the use of the model for mesoscale research applications as well as in regulatory photochemical modeling studies. Relevant recent experience of AG staff with the MM5 include: Tesche and McNally (1993a-f; 1996b); McNally and Tesche (1996a,b,f; 1998c); and Tesche et. al (1997a; 1999a). |
| **Time and resource constraints may be considered.** | Use of the MM5 model is consistent with the Denver EAC project schedule and budget. |
| **Consistency of the model with what was used in adjacent regional applications should be considered.** | MM5has been applied in several recent photochemical modeling studies including the recent CRC Comparative Model Evaluation Study in Lower Lake Michigan, the SARMAP study in California, various stakeholder studies participating in the OTAG, EPA NOx SIP Call, and EPA Tier II/Sulfur modeling analyses, the Pittsburgh-Beaver Valley SIP, the Cincinnati-Hamilton SIP, and in a half dozen other regional ozone modeling studies. The system was successfully applied in the Peninsular Florida 8-hr Ozone Study, the Kansas City/Missouri 8-hr ozone modeling study and recent 8-hr ozone studies in Texas and Oklahoma. MM5 was also recently used for regional-scale modeling of the southeastern U.S., with emphasis on Atlanta, Birmingham, and the eastern Gulf Coast. It was used for the Gulf Coast Ozone Study and was employed by AG staff in the design of the Breton Aerometric Monitoring Program (BAMP) in the Gulf of Mexico. Alpine staff exercised MM5 in previous modeling for the RAQC in the Denver region as well (McNally and Tesche, 1997d; 1998). |

**Table 2-9.** Factors justifying CAMx as the photochemical model for the Denver EAC study.

| Consideration | Rationale for Selection |
|---|---|
| **Nature of air quality problem leading to non-attainment of the ozone NAAQS should first be assessed, and the selected model should have the attributes and capabilities consistent with the perceived nature of the problem.** | Based on an analysis of the observed aerometric data together with the CDPHE's review of recent climatological data sets in the Denver-Northern Front Range Region, the potential 8-hr ozone nonattainment problem in the Denver area includes both regional and local components and is strongly influenced by the complex meteorology of the region. The CAMx photochemical modeling system is well suited for this application in that its urban- and regional-scale grid nesting scheme appropriately addresses the various time and space scales relevant to the mesoscale processes involved in 8-hr ozone episodes. Utilizing meteorological inputs from a nested prognostic model (MM5), CAMx can directly simulate the local processes involved in 8-hr ozone problems together with the influence of imported ozone and precursor species from upwind (regional-scale) source regions. The use of detailed meteorological inputs and grid nesting will allow proper treatment of the mountain-valley winds, upslope-downslope density driven flows, and vertical mixing and cloud processes. The process-analysis, ozone source apportionment, and direct decoupled sensitivity analysis algorithms (DDM) in CAMx will allow a more rigorous evaluation of model performance and aid in diagnostic analysis. |
| **Availability, documentation and past performance should be satisfactory.** | The CAMx modeling system is publicly available at no cost. Full user documentation can be obtained from the website: www.camx.com The CAMx model has been widely evaluated by numerous groups in the U.S . The model is more scientifically advanced model than the urban guideline UAM-IV model (Russell and Dennis, 2000; Tesche et al., 1992) and has undergone extensive successful testing by a variety of groups (see, for example, Lurmann and Kumar, 1997; McNally and Tesche, 1998a, McNally et al., 1998a-c; Tesche and McNally, 1998a; Tesche et al., 1998c,e,f). Model performance has consistently been comparable to or better than that of other contemporary model such as the UAM-V, SAQM, and URM. |
| **Relevant experience of available staff and contractors should be consistent with choice of a model.** | The CAMx modeling will be performed by ENVIRON and AG staff who are thoroughly knowledgeable of the use of the model for regulatory photochemical modeling studies. Relevant recent experience with CAMx include: Emigh et al., (1997); McNally and Tesche (1997c,d; 1998b; 1999a); McNally, Tesche and Russell (1996); McNally et al., (1996; 1997; 1998a,b,c); Morris, Tesche and Lurmann (1999); Tesche and McNally (1998a,b; 1998g; 1999d); Tesche et al, (1997d, 1998c,g,h,e,f; 1999a,b); and Tesche, McNally and Loomis (1998b,f,g,h) |
| **Time and resource constraints may be considered.** | Use of the CAMx model is consistent with the Denver EAC project schedule and budget. |
| **Consistency of the model with what was used in adjacent regional applications should be considered.** | CAMx has been applied in several recent photochemical modeling studies including the CRC Comparative Model Evaluation Study in Lower Lake Michigan (Tesche et al., 2000), the OTAG, EPA NOx SIP Call, and EPA Tier II/Sulfur modeling analyses, the Pittsburgh-Beaver Valley SIP, the Cincinnati-Hamilton SIP, and more than two dozen other regional ozone modeling studies in the eastern U.S. The system was also used in the Kansas City/Missouri, Oklahoma, East Texas, and Peninsular Florida 8-hr ozone modeling studies. |

# 3.0 EPISODE SELECTION

Identification and selection of suitable episodes is crucial to an ozone modeling study. Accordingly, it is important that the process be properly carried out, consistent with EPA guidance on 8-hr ozone modeling. This chapter discusses the episode selection process for the Denver EAC study, largely performed by the CDPHE, and later supplemented with analyses performed by ENVIRON/Alpine Geophysics. The CDPHE published a report identifying the methods and procedures it used for identifying candidate 8-hr modeling episodes for use in the Denver EAC study. These methods and procedures, as well as the agency's recommendations, are summarized in this section. Further details may be obtained from the full CDPHE (2003) report.

The main components of the Denver episode selection process included:

> Identification of the policy and technical issues influencing episode selection for regulatory 8-hr ozone attainment modeling;

> An objective episode selection process based on: (a) analysis of historical air quality and meteorology in the region, (b) synthesis of past studies, and (c) the consideration of the conceptual nature of the types, character, and frequency of occurrence of 8-hr ozone episodes in the Denver-Northern Front Range region; and

> Development of a prioritized list of recommended episodes complete with supporting air quality and meteorological analyses of the preferred period(s).

We begin by summarizing the key policy and technical issues associated with 8-hr ozone episode selection, consistent with EPA's episode selection recommendations. Next, we summarize the specific technical steps taken by the CDPHE in identifying and evaluating candidate 8-hr ozone episodes for the study area. We then summarize the current conceptual understanding of the conditions that lead to elevated 8-hr ozone concentrations in the Denver region. Finally, we identify three proposed modeling episodes – subsumed within a broader two-month window during the summer of 2002 -- that are recommended for the Denver EAC study.

## 3.1 EPA Guidance on 8-hr Ozone Episode Selection

The procedures for selecting 8-hr ozone modeling episodes, outlined in the EPA's draft guidance (EPA, 1999), seek to achieve a balance between good science and regulatory needs and constraints. Modeling episodes, once selected, influence technical and policy decisions for many years. Clearly, both the direct and implicit procedures used in selecting episodes warrant full consideration. The policy and technical issues that influenced episode selection for the Denver EAC study include:

> Selecting episode days with observed 8-hour ozone concentrations close to each monitors' Design Value and consistent with the form of the NAAQS (i.e. the ozone levels that lead to nonattainment designation);

> Representing the range of meteorological conditions that accompany exceedances of the 8-hour ozone standard;

> Selecting periods for which adequate emissions, air quality and meteorological data are available for model testing and application; and

> Accounting for the frequency of occurrence of the relevant aerometric conditions, appropriately excluding rare or extreme events.

Secondary criteria identified by EPA include (a) consideration of episodes modeled in recent, related studies if any; (b) observed concentrations "close" to the Design Value for as many monitoring sites as possible; (c) episodes representative of the current three-year period from which the Design Value is determined; and (d) episodes cover several adjacent nonattainment areas where feasible.

The main considerations governing the Denver EAC episode selection process involved (a) the episodes must be well suited for addressing the 8-hr ozone NAAQS; and (b) the data bases associated with the candidate episodes should be the best available to support the development of model inputs and the assessment of model performance. Table 3-1 lists several data base attributes that were also considered when assessing the suitability of potential modeling episodes.

Like most potential 8-hour ozone nonattainment areas around the U.S., the DNFRR has no high-resolution modeling data sets (e.g., VOC speciation data, aloft aerometric measurements) covering historical ozone episode periods. This is a significant limitation to regulatory modeling in the region and will limit to some degree the confidence RAQC decision-makers will ultimately be able to place on the modeling. Recognizing this limitation, it is vital that the episodes selected for modeling have the full complement of data from the existing routine meteorological and air quality monitoring networks. Thus, in selecting episodes, one should seek modeling periods with nearly complete routine measurement coverage.

## 3.2 CDPHE Selection Methodology

Typically, ozone modeling episode selection entails the following general activities: (a) define the technical and policy issues influencing selection of photochemical modeling episodes; (b) review findings of previous, relevant studies; (c) identify the detailed characteristics and frequency of occurrence of relevant meteorological regimes producing 8-hr ozone exceedances or near-exceedances; (d) assess the availability and adequacy of emissions, meteorological, and air quality data for developing model inputs and assessing model performance; and (e) rank-order the candidate episodes for modeling. The CDPHE's episode selection methodology generally incorporated these activities and supplemented them with the use of ozone forecast regression models that are routinely employed by the agency to perform summer ozone forecasting. These models use forecast upper level temperatures, winds, dew points and pressure level heights as well as ozone levels seen earlier in the period of interest to estimate peak current and next-day ozone concentrations. The models work well, although they tend to under predict the highest concentrations to some extent. These regression models proved useful in classifying ozone episodes based on the sensitivity of the regression parameter to the actual conditions.

### 3.2.1 CDPHE Episode Selection Procedure

The procedures employed by the CDPHE for selecting 8-hour ozone modeling episodes for the Denver area were as follows:

> Tabulate all days from 1999 to 2002 for which any ozone monitor in the six county area that had an 8-hour ozone concentration of 80 ppb or higher.

> Identify multi-day episode periods in which exceedances of the 8-hour ozone standard occurred for several days at monitors in the Denver area along with multiple monitors experiencing 8-hour ozone of 80 ppb or higher:

  - Eliminate days in which the 8-hour ozone exceedance is an isolated occurrence at one monitor with low ozone values at others;
  - Focus first on 8-hour ozone episodes for the Rocky Flats and NREL monitors whose ozone episodes are preferred due to historical high ozone.

> For each multi-day episode identified, summarize daily maximum 8-hour ozone concentrations at each Denver area monitor tabulating the number of exceedance days and high (> 80 ppb) 8-hour ozone days at each monitor.

> If meteorological data is available, perform back trajectory modeling from locations of 8-hour ozone exceedances during each candidate episode using the Hysplit model to:

  - Identify potential local versus transport ozone episodes;
  - Identify general direction of winds; and
  - Help classify the 8-hour ozone exceedance days into meteorological regimes.

> Select a subset of the most promising episodes as the final candidates that:

  - Have high and wide-spread 8-hour ozone concentrations with multiple exceedances in the Denver area;
  - Some candidate episodes also have high 8-hour ozone and 8-hour ozone exceedances in Weld County and in Rocky Mountain National Park;

- Represent the different types of meteorological conditions that lead to elevated 8-hour ozone concentrations in Denver, Weld County and Rocky Mountain National Park areas; and;

- Satisfy the EPA episode selection criteria listed above.

> Analyze the meteorological conditions of the final candidate 8-hour ozone episodes and develop a Conceptual Model of the ozone exceedance days.

Based on this approach, the available episodes were ranked for appropriateness for developing 8-hour ozone control plans for the Front Range. The CDPHE also made recommendations on which and number of episodes to be modeled to assure that all meteorological types associated with exceedances of the 8-hour ozone standard are captured.

### 3.2.2 Results of Historical Ozone Data Analysis

CDPHE examined monitored ozone data from the period of 1999-2002 to identify elevated 8-hour ozone episodes in the Denver metropolitan area. All days in which any ozone monitors in the Denver area that had a daily maximum 8-hour ozone concentration that was 80 ppb or higher were examined. Particular emphasis was placed on those ozone episodes that exceeded the 8-hour ozone standard (i.e., 85 ppb or higher for monitored concentrations).

The Colorado Department of Public Health and Environment operates 13 ozone monitors along the Front Range. Nine of these monitors are located in the Denver metropolitan area, with the other three in Colorado Springs, Ft. Collins, and Weld County. Highest ozone concentrations in the Denver area generally occur at monitors located along the foothills. Historically, the NREL monitor on Table Mountain in Golden and the Rocky Flats monitor in northern Jefferson County consistently record the highest levels. In addition, the Highland Reservoir and Chatfield monitors in Douglas County and the South Boulder Creek monitor in southern Boulder County have also recorded elevated concentrations. High ozone concentrations can occur on any day of the week, including weekends. Over the last five years, 69% of the 8-hour ozone levels above 75 ppb have occurred on weekdays while 31% have occurred on weekend days. Of the days above 90 ppb, 67% have occurred on weekdays and 33% on weekends. (Reference Reddy)

Table 3-2 summarizes the fourth maximum ozone values at all monitors in the state since 1996. The summer of 1998 had the highest ozone levels since 1996 with the fourth maximum levels at NREL and Rocky Flats above 90 ppb and values at several other monitors above 80 ppb. In 1999, 2000, and 2001, values were lower, with fourth maximum values less than 80 ppb at most monitors and in the low 80's for NREL and Rocky Flats.

Table 3-3 indicates the highest values at selected ozone monitors during the summer of 2002. There were three days in July (1st, 19th, and 20th) when ozone readings exceeded 90 ppb at one or more monitors in the region. The NREL monitor recorded values above 90 ppb on these three days and the fourth maximum value at the monitor was 81 ppb, which is consistent with historical levels at the monitor. The Rocky Flats monitor had an unusual pattern and number of high ozone days, when compared with other monitors during the summer of 2002.

While the monitor recorded a value above 90 ppb on July 19 when high values were recorded throughout the region, the monitor also recorded values in the high 80's on four days in early and late June, days when other monitors did not register exceptionally high values.

Table 3-4 summarizes the 3-year averages of fourth maximum values at selected monitors for 1998-2000 to 2000-2002. These values are comparable to the 8-hour ozone National Ambient Air Quality Standard (NAAQS). Because of the high values recorded in 2002, the Rocky Flats monitor has become the area of most concern since the 2000-02 average is 84 ppb, only one percent less than the violation level of 85 ppb. In 2003, the region would violate the standard if the 4th maximum at Rocky Flats were greater than 84 ppb as shown in Table 3-4 labeled as '2003 (Allow)'. There is greater cushion below the standard at the other monitors.

Elevated 8-hour ozone readings have also been recorded at times in Rocky Mountain National Park (RMNP). The highest ozone concentration in 2002 in the Park was 93 ppb, while the 4th maximum was 87 ppb. There were six days of monitored ozone values of 85 ppb or greater. Most of these days corresponded with days when high ozone concentrations were also recorded elsewhere in the Denver region. For five of these six days, 8-hour ozone concentrations in RMNP were as high as or higher than values in the remainder of the Denver region. During the previous four years, the high ozone concentrations in RMNP ranged from 80 ppb (2001) to 90 ppb (2000), while the annual fourth maximum values ranged from 70 ppb (2001) to 80 ppb (1998).

Table 3-5 presents a tabulation of all days that had a least one monitor with ozone concentrations greater than or equal to 80 ppb in the Denver area. Numbers in bold text are the maximum 8-hour ozone concentrations for the day. Shaded boxes in Table 3-5 are all additional 8-hour average ozone concentrations greater than 80 ppb. To the right of each date is the beginning hour of the 8-hour period for the maximum ozone concentration (bold text) for that day. Dates with boxes around them are potential episodes considered for meteorological and air quality modeling.

### 3.2.3 CDPHE Recommendations

As seen in Table 3-5, there were 51 days between 1999 and 2002 that had at least one monitor along the Front Range with an ozone concentration greater than or equal to 80 ppb. The highest concentration for a given day is identified in Table 3-5 in bold text. Ozone concentrations that are less than the maximum daily ozone concentration but greater than 80 ppb are identified by shaded boxes. During the 1999 to 2002 time frame, there were five episodes of two days or greater that can be used for episode selection. These episodes are identified in Table 3-5 with boxes drawn around the date. The five episodes recommended by the CDPHE (in priority order), are as follows:

- 18-21 July 2002
- 25 June-1 July 2002
- 8-12 June 2002
- 4-9 July 2001
- 3-4 August 2001

The first two episodes, 18-21 July 2002 and 25 June-1 July 2002 were viewed by CDPHE as equally important, although the possibility of exercising the models for the months of June-July (~60 days) was quite attractive since it would capture the top three episodes.

## 3.3 Summary of the Three Highest Ranked 8-hr Ozone Episodes

Detailed analyses for the top five episodes are discussed in the CDPHE (2003) report while here we summarize only the top three. Meteorological data for those days in the top three episodes were examined by CDPHE staff to see if there was a consistent or different type of meteorological regime that occurred that resulted in exceedance of the 8-hour ozone standard. Back trajectories were calculated by the CDPHE for each episode by using the NOAA HYSPLIT model (http://www.arl.noaa.gov/ss/models/hysplit.html). Back trajectories were calculated from the NREL site starting from the location of the 8-hour ozone exceedance and at three different heights above ground level (AGL): surface, 100-m, and 800-m. Different height levels allowed the for the assessment of the transport of low-level air parcels into the area as well as air parcels aloft above ground level. It also provided an indication of the level of wind shear in the atmosphere.

### 3.3.1 July 18-21, 2002

The highest ozone levels recorded at Rocky Flats North and NREL over the 1999 through 2002-time period characterized this episode. NREL recorded an 8-hour ozone concentration of 92 ppb on July 18. Rocky Flats North recorded a high 8-hour ozone concentration of 92 ppb on July 19. On July 19, seven monitors had monitored concentrations over 84 ppb including Highlands Ranch (86 ppb), South Boulder County (86 ppb), Chatfield (89 ppb), Rocky Flats North (92 ppb), NREL (91 ppb), and Rocky Mountain National Park (92 ppb). Two monitors, Carriage (83 ppb) and Arvada (84 ppb) had 8-hour ozone concentration greater than 80 ppb but less than 85 ppb.

This period had nine days of temperatures greater than or equal to 90 degrees F. from July 12 through July 20$^{th}$. On the last day of the episode (July 21) the temperature made it up to 85 degrees. Dryness, subsidence, and stable conditions predominated the episode. An upper level ridge was centered over Colorado. This ridge was nearly stationary for several days. Despite southeast surface flow along the Front-Range, dew point levels were low enough to inhibit thunderstorm activity. There was some thunderstorm activity in the mountains, though.

On Thursday, July 18$^{th}$, there was a slight increase in mid-level moisture during the day. There was too much stability in the atmosphere for thunderstorm development despite the increase in moisture. The strength of the upper ridge peaked on Friday, January 19. The peak strength of the upper ridge coincided with the highest area wide ozone concentrations. Eastern Colorado appeared to be in a dry subsident hole as subtropical moisture extended from Mexico north into Utah and southern Canada. On Saturday, July 20, a quick moving Canadian/Pacific short wave pushed through Montana and North Dakota. The result of this short wave weakened the northern section of the upper ridge. Subtropical moisture migrated over eastern Colorado. Northeastern Colorado began to see stronger diurnal east to northwest surface flow late on Saturday. The diurnal surface flow was enhanced by rising surface heights overnight.

The ozone episode essentially ended on Sunday, July 21. A short wave crossed the northeastern Colorado plains during the early morning hours with some rain shower activity. The effect of this short wave was to suppress afternoon convective activity. A second, weaker short wave crossed over northeastern Colorado during the afternoon hours. Some shower activity in Larimer and Weld Counties resulted from the passage of the second short wave. For the most part, cooler temperatures resulting from a moist and cooler northeasterly flow suppressed convective activity. Winds aloft were also weak during the day, and, for most of the episode as well.

Backward trajectories were computed for July 17 through July 21, 2002. These composite backward trajectory analyses indicated that at lower levels up to 100 meters, the origin of the air mass was from the south and east during the early days of the episode and then from the north during the late part of the episode. Upper layers of flow were from the northwest and may have originated from Salt Lake City but this may be misleading as the 36-hour back trajectories were from the south. Thirty-six hour trajectories for each day indicated that the Northwesterly flow might be an artifact of the long period the trajectory analysis was ran. The mid-level air mass was mixed down to ground level by the time it reached the Denver area. The flow from the various layers (surface, 100m, and 800m) were generally from the south. Flow at 800 m was very light and did not mix down to the ground. Even at 100m the flow did not mix down to the ground either.

On July 19, the flow at all levels were again from the south. Winds speeds were less than the previous day and apparently the flow had a tendency to go around the Palmer Divide. The 800m winds did not mix down to ground level but flowed over the Palmer Divide. On July 20, when NREL had its highest reading over the episode, the ground level flow was very light from the west. There is some indication that flow in the lower levels circulated along the front range. The flow on this day very likely brought in smoke from the Big Elk Fire that was burning near Estes Park. At the 800m level, the flow was from the south over the Palmer Divide. The general flow shifted on the last day of the episode. Winds at the surface were from the north. At the 800m level, winds were from the northwest.

### 3.3.2 25 June-July 1, 2002

This episode was lengthy when compared to the other episodes. There were seven days in a row where at least one monitor exceeded 80 ppb. This episode had the highest 8-hour average ozone concentration recorded at Rocky Mountain National Park of 93 ppb recorded on June 30. Three days had at least one monitored concentration that exceeded 85 ppb. On June 29, Rocky Flats North recoded an 8-hour average concentration of 89 ppb. However the rest of the monitors in the network had values less than 80 ppb on this date. On June 30, Rocky Mountain National Park recorded a 93 ppb and Rocky Flats north recorded a value of 88 ppb. Both NREL and South Boulder County had 8-hour ozone concentrations of 80 ppb.

The highest ozone concentration occurred in southwest Denver on July 1 where Chatfield recorded a value of 94 ppb. This is the highest ozone concentration recorded over the entire network during the 1999-2002 periods. Highlands Ranch also exceeded the 8-hour ozone concentration at 86 ppb. Values greater than 85 ppb were also recorded at Rocky Flats North (88 ppb), NREL (91 ppb), and Rocky Mountain National Park (85 ppb). A value of 82 ppb was recorded at the Weld County Tower. It should be noted that several large wildfires were burning during this period including the Rodeo Fire in Arizona, the Mission Ridge Fire near Durango, the Hayman Fire near Denver, and other fire complexes in western Colorado. Flow during the later parts of this episode, as indicated by the trajectory plots, blew from one or more of these large fires.

A stretch of 13 consecutive days of 90 degree F or more occurred from June 21 through July 3. The maximum temperature exceeded 95 degrees F on June 26 (96°F), June 29 (97°F), and July 1 (99°F). On June 25, a warm upper ridge dominated the southwest United States including Colorado through the period. Mid-level winds were weak north to easterly (upslope) to about 700 mb. Surface dew points were fairly moist at 40 to 50 degrees F. Winds aloft were weak and convective storm motion was slow. The upper level ridge remained intact along the Rockies from Mexico to southern Canada on June 26. Winds from the surface to 600 mb were light and from the east. The eastern plains had a fairly moist air mass (50 degree F dew points) but the stable atmosphere prevented much in the way of thunderstorms on the plains. Cooler air had advected into the 700 to 500 mb levels. Surface winds to 700 mb were more northly and a bit stronger than the day before. The upper level ridge was slightly weaker than the day before and more disorganized but little movement was detected. Winds aloft were weak with slow moving convective storms.

The high-pressure ridge was again in control of the state on June 27. Surface southeast flow on the plains provided for slightly drier air. Convective storms that developed in the mountains died off quickly over the drier and capped air mass over the plains. Friday, June 28 continued the same weather pattern. The air mass was dry and capped over the eastern plains. Any convective storms that developed over the mountains, quickly dissipated over the eastern plains except for a few very slow moving storms. Heavy rain occurred in some areas because of the slow moving storms. The Platteville profiler indicated light and variable winds from the surface on up.

A convergence zone formed from southeastern Douglas County through eastern Adams County on the afternoon of Saturday, June 29. The convergence zone separated very dry air coming off of the foothills from moist (45-55 degree F) dew points to the south and east. Flow aloft was stronger and more organized than on previous days. The flow aloft was also more from the west and northwest than on the previous days. Despite a dry cold front sliding southward through eastern Wyoming, overnight temperatures did not fall much below 70 degrees F until the early morning hours.

Sunday, June 30 and Monday, July 1 had the highest ozone concentrations over the episode. On Sunday, the air mass over northeastern Colorado was very dry and stable following the cold front passage. Subsidence from the already warm and dry air mass pushed temperatures near the century mark over much of eastern Colorado. A mid-level inversion prevented any thunderstorms from building on the eastern plains. Moderate levels of smoke from several fires burning in the west (Hayman, Missionary Ridge, Rodeo in Arizona, and Million Fire) were reported along the northern Front Range. Monday, July 1 was more of the same. Strong mid-level subsidence over the northeastern plains continued to dominate the local weather pattern. High ozone readings were widespread over the network. Ozone levels decreased on July 2 and 3 with temperature continuing over 90 degrees F. Gulf moisture moved into the area across the mountains and foothills. A weak cap around 500 mb was still present over the area. Surface winds shifted to the northeast. No real strong indications why the ozone episode did not continue on July 2 and 3.

This episode was strongly influenced by flow from the southwestern United States including southern California and Arizona. Subsidence over Colorado mixes surface and 800m layers down to the surface by the time they reach the Front Range. The flow from June 25 through June 28 was generally from the south. Winds during this period were light at all levels, especially on June 25. During this period, ozone concentrations were the lowest during the episode. On June 28, winds became stronger from the south. Upper levels winds at 800m started to shift from the southwest. On June 29 through July 1, winds at 800m were from the southwest, originating in Arizona and Utah. Surface winds were light during this period originating from the west and southwest.

### 3.3.3 8-12 June 2002

This period occurred just three days after the start of the Hayman fire. Very warm temperatures along with smoky conditions characterized this episode. Concentrations of 88 ppb occurred on two days, June 8 and 9, at Rocky Flats North. A value of 88 ppb were recorded at NREL on June 9 as well. A value of 83 ppb occurred at Rocky Mountain National Park on June 11 and at Rocky Flats North on June 12. During this episode, other monitors in the network were all below 80 ppb indicating that this episode was not widespread.

June 8 and 9, when the highest ozone readings occurred, the maximum temperature reached 96 degrees F and 95 degrees F, respectively. Despite cooler temperature on June 11 and 12, ozone readings above 80 ppb were monitored on these days. The maximum temperatures recorded on June 11 and 12 were 78 degrees F and 82 degrees F, respectively. Ozone readings were below 80 ppb on June 10 when the maximum-recorded temperature was 75 degrees F. On June 8, shallow moist air covered most of eastern Colorado during the morning hours. This moist air mass mixed out as the day progressed. Very little convective activity occurred over the mountains and northeastern plains. Smoke from the Hayman fire was observed over the Denver area on June 9. A weak short wave passed north of the area during the evening hours. As a result of the short wave passage, winds aloft shifted to a westerly direction. The inversion layer lowered to about 2000 feet overnight.

Much colder air moved into the area on June 10 with the maximum temperature in Denver recorded at 75 degrees F. Consequently, no ozone readings exceeded 80 ppb. Winds had shifted to the southeast for most of the day. An inversion persisted for most of the day on June 11. The height of the inversion was around 18 thousand feet. Although ozone readings were low network wide, Rocky Mountain National Park had a reading of 83 ppb. An ozone reading of 83 ppb was recorded at Rocky Flats north on June 12. Except for smoke in the area from the Hayman Fire, very little else can be said about this day. Warm temperatures over the mountains with cooler temperatures over the plains were indicative of a persistent inversion over the area.

The composite trajectory analyses revealed that the air parcels originated in very different areas at the three levels over the 120-hour simulation. At the surface, the flow was from the south from Texas, at 100m the flow was from the southwest from Arizona, and at 800m the flow was from the northwest from Salt Lake City. The 36- hour plots indicated the flow was from the southwest from Arizona on June 8th through June 10th at all levels. The southwesterly flow was fairly strong originating in Arizona and southern California at the start of each 36-hour period. On June 11 and 12, the flow became more westerly at 800m. The surface flow was from the Nebraska panhandle on June 11. The northeasterly flow was much less on this date. By June 12 the surface flow had shifted to the southwest with fairly light wind speeds.

## 3.4 Strengths and Limitations of Recommended 8-hr Ozone Modeling Episodes

Based on EPA's episode selection criteria, the CDPHE identified the main advantages and disadvantages for the three highest priority episodes.

### 3.4.1 July 18-21, 2002

Advantages:

- Somewhat contains three different types of regimes:
  - July 18-19 there was a southerly flow from source types like Texas and New Mexico
  - A localized scenario occurred on July 20 when surface winds were very light. This day may also be used to evaluate the effects of wildfire since winds were consistent from those coming from the Big Elk Fire near Estes Park
  - Northerly flow on July 21 from Wyoming where the effects of flash emissions to Denver ozone could be evaluated

- Contains the highest ozone concentrations at the key receptors NREL (92 ppb) and Rocky Flats North (92 ppb) over the four year period as demonstrated in Table 3-5.

- Contains the second highest ozone concentration at Rocky Mountain National Park (92 ppb)

- Table 3-6 shows that the average over the episode at Rocky Flats North (81 ppb) is very close to the average of the fourth highs for 2000-2002 (84 ppb). This is also the case for South Boulder Cr., Highlands, and Chatfield. Although the episode high for NREL is slightly higher than the average of the fourth highest concentrations in 2000-2002, it is consistent with the average of the fourth highest concentrations in 1998-2000.

- The wide spread network exceedances on July 19 provides a basis for demonstrating attainment at all of the Denver metro monitors. On July 19, eight out of the 12 Front Range monitors exceeded 80 ppb. This is back up on the follow day, July 20, when 6 monitors were 80 ppb or greater.

Disadvantages

> Four days is a short duration episode

> Possibly contains smoke and ozone precursor emissions from the Big Elk Fire near Estes Park

### 3.4.2 June 25 – July 1, 2002

Advantages

> Contains the longest string of days when the monitoring network exceeded 80 ppb

> The highest ozone concentration recorded during the 2000-2002 period occurred at Highlands on July 1 with a concentration of 94 ppb

> The highest ozone concentration occurred at Rocky Mountain National Park on June 30 with a value of 93 ppb.

> The last three days of the episode had high ozone concentrations (greater than 85 ppb) Rocky Flats North (89 ppb, 88 ppb, and 88 ppb, respectively). A high ozone concentration (91 ppb) was also monitored at NREL on July 1

> Contains a consistent southerly flow from southern Colorado during the first three days. Contains a second scenario type with southwesterly flow from Arizona and Southern California.

> On June 30, 4 out of 12 monitors were greater than 80 ppb. On July 1, 5 out of 12 monitors exceeded 80 ppb. However, the exceedances were at key monitors.

> Table 3-7 shows that the average over the episode at Rocky Flats North (84 ppb) is the same as the average of the fourth highs for 2000-2002 (84 ppb). The episode average is also very close to the average fourth high values at other key receptors.

Disadvantages

> The first three days of the episode had fairly low (below 85 ppb) ozone concentrations over the entire network

> Rocky Flats North did not operate on June 25 and 26.

> Several large wildfires were burning in the southwest and Rockies including the Rodeo fire in Arizona, Missionary Ridge fire near Durango, fire complexes near the Utah and Colorado border, and fire complexes near Steamboat Springs. It would be hard to inventory these fires and to evaluate their effects on Denver ozone.

### 3.4.3 June 8 – 12, 2002

Advantages

> Concentrations at Rocky Flats North were 88 ppb on two of the episode days (June 8 and 9) which contributes significantly to the average of the fourth highest concentrations between the 2000-2002 period.

> Good case study to evaluate the effects of wildfire on ozone and particulate matter levels.

> Good case study for evaluating the effects of transport from Arizona and Southern California (June 8-10)

> An equally good case study for evaluating the local production of ozone and transport of ozone from the eastern plains of Colorado (June 11 and 12)

Disadvantages

> Episode occurred just three days after the start of the Hayman fire. It would be hard to create an inventory for this fire and to model its effect on ozone over the Denver area.

> Table 3-8 shows that the average over the episode at Rocky Flats North (84 ppb) is close to the average of the fourth highs for 2000-2002 (84 ppb). However, at other key receptors line NREL the episode average is far below the average of the fourth highest concentrations.

> There were not widespread ozone concentrations greater than 80 ppb over the entire network.

> Similar to the episode that occurs on June 25 through July 1, 2002

## 3.5 Summary of the Conceptual Model of 8-hr Ozone Episodes for the DNFRR

The CDPHE developed a succinct conceptual model of 8-Hour Ozone formation in the Denver Northern Front Range Region (CDPHE, 2003). Salient features of the model are as follows. High ozone concentrations generally occur in the Denver region on days that are hot, cloud-free, and with stagnant to light wind speeds at both at the surface and aloft. Most high-ozone events occur on days when high temperatures are above 90 degrees F and when light, up-slope winds occur at the surface and mountaintop level. Episodic events of ozone occur when maximum daily temperatures above 90 degrees F persist for several days in a row. On most high ozone days, dew points on the eastern plains are in the 40-60 $^{O}$F range. Relatively high dew point levels are probably necessary for efficient photochemistry production and differentiate those days that are above 90 $^{O}$F with high ozone levels, and, dry hot days with lower ozone levels. The absence of cloud cover and thunderstorms promotes ozone formation. Conversely, typical late-afternoon thunderstorms and associated cloud cover retard the formation of ozone and help keep ozone concentrations at levels below the federal standard. Timing of thunderstorms off of the mountains in the late afternoon and evening hours during hot days is another critical piece in determining whether the 8-hour ozone standard is exceeded on a day-to-day basis in the Denver area. The highest ozone levels usually occur in June and July and sometimes-early August.

## 3.6 Recommended Summer ’02 Episode and Intensive Study Periods

Based on discussions with the RAQC and CDPHE during the project kickoff meeting, it was agreed that the Denver 8-hr ozone study would focus on the three 2002 episodes as a single MM5/CAMx regional simulation. We call this the ‘Summer ‘02’ episode which runs from 5 June to 23 July 2002. Meteorological inputs from the MM5 model will be produced on the 36/12 km grid for the period beginning 1200 UTC (0500 MST) on 5 June 2002 through 1200 UTC (0500 MST) on 23 July 2002. The higher resolution MM5 simulations will be active during the following periods:

- 1200 UTC (0500 MST) on 16 July through 1200 UTC (0500 MST) on 23 July;
- 1200 UTC (0500 MST) on 23 June through 1200 UTC (0500 MST) on 3 July; and
- 1200 UTC (0500 MST) on 5 June through 1200 UTC (0500 MST) on 14 June.

The CAMx model will be run at 12km resolution from 0000 MST on 7 June through midnight on 22 July 2002. The higher resolution 4 km and 1.33 km CAMx grid nests will be run from:

- 0000 MST on 8 June through 2400 MST on 12 June (i.e., 8-12 June);
- 0000 MST on 25 June through 2400 MST on 1 July (i.e., 25 June-1 July); and
- 0000 MST on 18 July through 2400 MST on 21 July 2002 (i.e., 18-21 July).

These latter two intensive study periods are the top two ranking episodes in the CDPHE’s ozone episode selection scheme. As indicated previously, the 8-12 June episode is potentially confounded by the presence of major wildfires throughout the western states. Accordingly, we propose to include the 8-12 June period within the overall Summer ’02 modeling episode. However, we make the following cautionary note. Should it be determined that the uncertainties in the modeling of the 8-12 June 2002 episode are unacceptability large owing to the wildfires (thereby precluding reliable source-receptor modeling), this intensive period may not be used to assess compliance with the 8-hr ozone standard. In this eventuality, the other two episodes would be used for this purpose.

**Table 3-1.** Episode attributes that should be qualitatively reviewed during an ozone modeling episode selection process.

| Episode Attribute | Description |
|---|---|
| Synoptic and Mesoscale Overview | The synoptic and mesoscale meteorological conditions should be representative of those conditions that produce ozone episodes. |
| Classification and Frequency of Ozone Episode Class | The episode should be typical of climatological ozone episodes that occur with sufficient frequency of magnitude to be of regulatory significance. |
| Ozone Maxima of Regulatory Significance | The ozone maxima during the episode should be of sufficient magnitude that the episode can serve as a “design day” for developing a control strategy. |
| Representativeness of Design Monitor | The peak monitoring site, or sites, should be representative of regional ozone levels and not ozone levels produced by nearby emissions or local meteorological conditions. |
| Absence of Unusual Diurnal Concentration Trends | Ozone and precursor pollutant concentrations should follow normal or typical diurnal trends in both timing and magnitude. |
| Coherence of Surface Wind Patterns | The surface winds should produce relatively steady-state, consistent, and predictable flow patterns throughout the modeling domain. |
| Coherence of Aloft Wind and Thermal Patterns | The aloft thermal stratifications and wind flow should be dynamically consistent over the study area and not be the result of unusual mesoscale or synoptic meteorological conditions. |
| Data Availability for Initial/Boundary Conditions | Adequate surface and aloft data should exist to specify ozone and precursor pollutant concentrations at the beginning of the episode (initial conditions) and at the lateral and top inflow boundaries of the modeling domain (boundary conditions). |
| Data Availability for Ozone and Performance Evaluation | The number and coverage of ozone monitors should be such that the temporal and spatial resolution of these data are adequate to conduct a performance evaluation of ozone predictions made by the photochemical model. |
| Data Availability for Multi-Species Testing | The number and coverage of non-ozone precursor pollutant species should be such that the temporal and spatial resolution of theses data are adequate to conduct a performance evaluation of precursor pollutant species predictions made by the photochemical model. |
| Data Completeness | The minimum acceptable set of meteorological and air quality parameters needed for use in preparing model emission, meteorological and photochemical model inputs should be available. |
| Desired Prototypical Behavior | The episode should display the desired source-receptor relationships that are required to allow assessment of alternative control strategies, including both “locally-generated” ozone and “regionally-transported” ozone. |
| Ability of Episode and Data Base to “Stress” Models | The episode should have sufficient data to support “stress-testing” of the model. |
| Prospects for Successful Modeling | There should be a reasonable chance of success in producing an acceptable model performance evaluation for the episode. |
| Computational and Schedule Considerations | The modeling analysis should be able to be completed in an acceptable period of time and with available computer resources. |

**Table 3-2.** Fourth maximum 8-hour ozone concentrations from 1996 through 2002 (Source: CDPHE, 2003).

| Site Name | 1996 8-hr O3 4th Max. (ppm) | 1997 8-hr O3 4th Max. (ppm) | 1998 8-hr O3 4th Max. (ppm) | 1999 8-hr O3 4th Max. (ppm) | 2000 8-hr O3 4th Max. (ppm) | 2001 8-hr O3 4th Max. (ppm) | 2002* 8-hr O3 4th Max. (ppm) |
|---|---|---|---|---|---|---|---|
| Welby | 0.074 | 0.071 | 0.083 | 0.071 | 0.062 | 0.064 | 0.068 |
| Highland | 0.073 | 0.065 | 0.084 | 0.075 | 0.076 | 0.077 | 0.076 |
| S. Boulder Creek | 0.075 | 0.072 | 0.089 | 0.075 | 0.072 | 0.071 | 0.078 |
| Carriage | .0.068 | 0.066 | 0.085 | 0.068 | 0.071 | 0.072 | 0.073 |
| Chatfield Res. | 0.079 | 0.075 | 0.081 | 0.075 | 0.080 | 0.077 | 0.083 |
| USAF Academy | 0.057 | 0.059 | 0.062 | 0.064 | 0.072 | 0.070 | 0.072 |
| Arvada | 0.073 | 0.070 | 0.089 | 0.072 | 0.076 | 0.074 | 0.073 |
| Welch | 0.069 | 0.068 | 0.080 | 0.066 | 0.068 | 0.064 | 0.069 |
| Rocky Flats North | 0.083 | 0.076 | 0.092 | 0.080 | 0.081 | 0.082 | 0.088 |
| NREL | 0.082 | 0.075 | 0.092 | 0.080 | 0.083 | 0.081 | 0.081 |
| Fort Collins | 0.066 | 0.064 | 0.072 | 0.063 | 0.070 | 0.067 | 0.072 |
| Greeley | 0.070 | 0.069 | 0.075 | 0.069 | 0.069 | 0.074 | --- |
| Weld County Tower | --- | --- | --- | --- | --- | --- | 0.080 |

Data through August 2002

**Table 3-3.** Highest ozone concentrations at selected monitors-2002. (Source: CDPHE, 2003).

| Monitor | 1st Max | 2nd Max | 3rd Max | 4th Max |
|---|---|---|---|---|
| NREL | 20-Jul | 19-Jul | 1-Jul | 18-Jul |
| | **0.092** | **0.091** | **0.091** | **0.091** |
| Rocky Flats | 19-Jul | 29-Jun | 8-Jun | 9-Jun** |
| | **0.092** | **0.089** | **0.088** | **0.088** |
| S. Boulder Creek | 19-Jul | 30-Jun | 9-Jun | 29-Jun |
| | **0.086** | **0.080** | **0.079** | **0.078** |
| Highlands Res. | 1-Jul | 19-Jul | 12-Jun | 28-Jun |
| | **0.086** | **0.086** | **0.076** | **0.076** |
| Chatfield Res. | 1-Jul | 19-Jul | 28-Jun | 20-Jul |
| | **0.094** | **0.089** | **0.083** | **0.083** |
| ** Another 0.088 ppm level was recorded on 6/30/02 | | | | |

**Table 3-4.** Three-year average of 4th maximum values (ppm)-1998-2002. (Source: CDPHE, 2003).

| Site Name | 1998 | 1999 | 2000 | 2001 | 2002 | 98-00 Average | 99-01 Average | 00-02 Average | 2003 (Allow) |
|---|---|---|---|---|---|---|---|---|---|
| NREL | 0.095 | 0.080 | 0.083 | 0.081 | 0.081 | 0.086 | 0.081 | 0.082 | 0.092 |
| Rocky Flats-N | 0.092 | 0.080 | 0.081 | 0.082 | 0.088 | 0.084 | 0.081 | 0.084 | 0.084 |
| South Boulder Cr. | 0.089 | 0.075 | 0.072 | 0.071 | 0.078 | 0.078 | 0.073 | 0.074 | 0.105 |
| Highlands | 0.084 | 0.075 | 0.076 | 0.077 | 0.076 | 0.078 | 0.076 | 0.076 | 0.101 |
| Chatfield | 0.081 | 0.075 | 0.080 | 0.077 | 0.083 | 0.079 | 0.077 | 0.080 | 0.094 |

**Table 3-5.** Day with at least one monitored ozone concentrations greater than or equal to 80 ppb in the Denver area. (Source: CDPHE, 2003).

| | Hour of Max. | Welby Daily Max Sample Value | Highland Daily Max Sample Value | S. Bldr. Crk. Daily Max Sample Value | Carriage Daily Max Sample Value | Chatfield Daily Max Sample Value | Academy Daily Max Sample Value | Arvada Daily Max Sample Value | Welch Daily Max Sample Value | RFN Daily Max Sample Value | NREL Daily Max Sample Value | NPS Daily Max Sample Value | Ft. Collins Daily Max Sample Value | Greeley Daily Max Sample Value | WCTower Daily Max Sample Value |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 09-APR-1999 | 13 | 0.069 | 0.075 | 0.038 | 0.069 | N / A | 0.081 | 0.068 | 0.068 | 0.072 | N / A | 0.073 | 0.062 | 0.062 | N / A |
| 06-MAY-1999 | 9 | 0.075 | 0.075 | 0.070 | 0.062 | 0.076 | 0.068 | 0.070 | 0.067 | 0.078 | N / A | 0.085 | 0.071 | 0.071 | N / A |
| 26-JUN-1999 | 10 | 0.064 | 0.072 | 0.063 | 0.062 | 0.079 | 0.054 | 0.068 | 0.064 | 0.073 | 0.080 | 0.056 | 0.055 | 0.059 | N / A |
| 01-JUL-1999 | 12 | 0.061 | 0.058 | 0.075 | 0.063 | 0.061 | 0.045 | 0.069 | 0.061 | 0.087 | 0.078 | 0.038 | 0.059 | 0.052 | N / A |
| 06-JUL-1999 | 11 | 0.066 | 0.056 | 0.071 | 0.065 | 0.059 | 0.047 | 0.067 | 0.059 | 0.077 | 0.081 | 0.042 | 0.051 | 0.048 | N / A |
| 07-JUL-1999 | 9 | 0.069 | 0.067 | 0.077 | 0.065 | 0.065 | 0.051 | 0.072 | 0.058 | 0.081 | 0.076 | 0.056 | 0.066 | 0.066 | N / A |
| 13-JUL-1999 | 10 | 0.081 | 0.082 | 0.086 | 0.077 | 0.079 | 0.064 | 0.081 | 0.071 | 0.092 | 0.084 | 0.064 | 0.061 | 0.069 | N / A |
| 17-JUL-1999 | 10 | 0.070 | 0.069 | 0.068 | 0.065 | 0.069 | 0.049 | 0.072 | 0.059 | 0.075 | 0.080 | 0.063 | 0.058 | 0.058 | N / A |
| 27-JUL-1999 | 11 | 0.068 | 0.068 | 0.083 | 0.068 | 0.069 | 0.054 | 0.076 | 0.065 | 0.081 | 0.085 | 0.063 | 0.057 | 0.066 | N / A |
| 28-JUL-1999 | 9 | 0.071 | 0.080 | 0.067 | 0.072 | 0.075 | 0.070 | 0.069 | 0.064 | 0.071 | 0.076 | 0.061 | 0.052 | 0.073 | N / A |
| 26-AUG-1999 | 10 | 0.069 | 0.081 | 0.063 | 0.066 | 0.077 | 0.054 | 0.061 | 0.060 | 0.075 | 0.077 | 0.065 | 0.049 | 0.059 | N / A |
| 16-MAY-2000 | 12 | 0.066 | 0.053 | 0.067 | 0.069 | 0.054 | 0.045 | 0.076 | 0.049 | 0.082 | 0.075 | 0.068 | 0.062 | 0.026 | N / A |
| 30-JUN-2000 | 14 | 0.055 | 0.062 | 0.066 | 0.063 | 0.059 | 0.062 | 0.061 | 0.049 | 0.071 | 0.070 | 0.089 | 0.063 | 0.052 | N / A |
| 10-JUL-2000 | 11 | 0.058 | 0.067 | 0.053 | 0.069 | 0.065 | 0.063 | 0.072 | 0.048 | 0.075 | 0.081 | 0.067 | 0.052 | 0.059 | N / A |
| 15-JUL-2000 | 8 | 0.062 | 0.085 | 0.063 | 0.064 | 0.083 | 0.067 | 0.070 | 0.071 | 0.077 | 0.081 | 0.068 | 0.065 | 0.060 | N / A |
| 16-JUL-2000 | 11 | 0.058 | 0.069 | 0.058 | 0.065 | 0.067 | 0.059 | 0.070 | 0.067 | 0.072 | 0.082 | 0.062 | 0.054 | 0.053 | N / A |
| 20-JUL-2000 | 10 | 0.056 | 0.076 | 0.061 | 0.069 | 0.080 | 0.051 | 0.076 | 0.072 | N / A | 0.084 | 0.063 | 0.051 | 0.049 | N / A |
| 28-JUL-2000 | 10 | 0.062 | 0.086 | 0.066 | 0.076 | 0.080 | 0.068 | 0.079 | 0.068 | 0.084 | 0.089 | 0.076 | 0.068 | 0.062 | N / A |
| 01-AUG-2000 | 12 | 0.053 | 0.076 | 0.066 | 0.067 | 0.078 | 0.069 | 0.068 | 0.070 | 0.079 | 0.083 | 0.086 | 0.059 | 0.064 | N / A |
| 02-AUG-2000 | 10 | 0.050 | 0.072 | 0.066 | 0.071 | 0.080 | 0.081 | 0.061 | 0.066 | 0.075 | 0.083 | 0.078 | 0.069 | 0.071 | N / A |
| 09-AUG-2000 | 10 | 0.055 | 0.066 | 0.078 | 0.057 | 0.069 | 0.064 | 0.063 | 0.058 | 0.081 | 0.066 | 0.080 | 0.070 | 0.063 | N / A |
| 13-AUG-2000 | 10 | 0.054 | 0.067 | 0.077 | 0.069 | 0.073 | 0.068 | 0.070 | 0.068 | 0.077 | 0.080 | 0.069 | 0.077 | 0.076 | N / A |
| 15-AUG-2000 | 12 | 0.062 | 0.074 | 0.075 | 0.078 | 0.076 | 0.072 | 0.078 | 0.066 | 0.083 | 0.081 | 0.075 | 0.050 | 0.064 | N / A |
| 16-JUN-2001 | 13 | 0.056 | 0.057 | 0.073 | 0.067 | 0.069 | 0.051 | 0.071 | 0.061 | 0.083 | 0.077 | 0.042 | 0.057 | 0.055 | N / A |
| 01-JUL-2001 | 9 | 0.062 | 0.064 | 0.061 | 0.058 | 0.072 | 0.053 | 0.072 | 0.063 | 0.073 | 0.081 | 0.042 | 0.070 | 0.084 | N / A |
| 04-JUL-2001 | 8 | 0.066 | 0.064 | 0.064 | 0.072 | 0.075 | 0.057 | 0.077 | 0.063 | 0.081 | 0.076 | 0.045 | 0.064 | 0.081 | N / A |
| 05-JUL-2001 | 10 | 0.062 | 0.080 | 0.069 | 0.072 | 0.089 | 0.069 | 0.078 | 0.063 | 0.087 | 0.081 | 0.045 | 0.067 | 0.064 | N / A |
| 07-JUL-2001 | 10 | 0.063 | 0.073 | 0.071 | 0.073 | 0.076 | 0.065 | 0.074 | N / A | 0.081 | 0.083 | 0.063 | 0.060 | 0.074 | N / A |
| 09-JUL-2001 | 11 | 0.065 | 0.071 | 0.060 | 0.066 | 0.077 | 0.070 | 0.040 | 0.064 | 0.084 | 0.075 | 0.058 | 0.055 | 0.081 | N / A |
| 03-AUG-2001 | 12 | 0.054 | 0.077 | 0.076 | 0.051 | 0.075 | 0.065 | 0.062 | 0.061 | 0.082 | 0.067 | 0.080 | 0.064 | 0.070 | N / A |
| 04-AUG-2001 | 11 | 0.063 | 0.082 | 0.071 | 0.078 | 0.083 | 0.066 | 0.083 | 0.080 | 0.081 | 0.090 | 0.061 | 0.059 | 0.063 | N / A |
| 08-JUN-2002 | 12 | 0.065 | 0.060 | 0.066 | 0.069 | 0.062 | 0.064 | 0.074 | 0.056 | 0.088 | 0.078 | 0.073 | 0.082 | N / A | 0.077 |
| 09-JUN-2002 | 12 | 0.057 | 0.060 | 0.079 | 0.059 | 0.057 | 0.059 | 0.069 | 0.051 | 0.088 | 0.073 | 0.088 | 0.068 | N / A | 0.073 |
| 11-JUN-2002 | 12 | 0.054 | 0.059 | 0.062 | 0.044 | 0.060 | 0.056 | 0.053 | 0.045 | 0.068 | 0.058 | 0.083 | 0.064 | N / A | 0.066 |
| 12-JUN-2002 | 13 | 0.069 | 0.076 | 0.071 | 0.059 | 0.075 | 0.067 | 0.072 | 0.055 | 0.083 | 0.074 | 0.077 | 0.067 | N / A | 0.071 |
| 25-JUN-2002 | 8 | 0.059 | 0.058 | 0.068 | 0.068 | 0.061 | 0.056 | 0.065 | 0.060 | 0.080 | 0.075 | 0.075 | 0.070 | N / A | 0.070 |
| 26-JUN-2002 | 12 | 0.068 | 0.074 | 0.073 | 0.073 | 0.079 | 0.071 | 0.068 | 0.065 | N / A | 0.077 | 0.077 | 0.073 | N / A | 0.081 |

| | Hour of Max. | Welby Daily Max Sample Value | Highland Daily Max Sample Value | S. Bldr. Crk. Daily Max Sample Value | Carriage Daily Max Sample Value | Chatfield Daily Max Sample Value | Academy Daily Max Sample Value | Arvada Daily Max Sample Value | Welch Daily Max Sample Value | RFN Daily Max Sample Value | NREL Daily Max Sample Value | NPS Daily Max Sample Value | Ft. Collins Daily Max Sample Value | Greeley Daily Max Sample Value | WCTower Daily Max Sample Value |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 27-JUN-2002 | 11 | 0.062 | 0.071 | 0.073 | 0.066 | 0.075 | 0.073 | 0.065 | 0.062 | N / A | 0.071 | 0.081 | 0.068 | N / A | **0.081** |
| 28-JUN-2002 | 9 | 0.064 | 0.077 | 0.065 | 0.071 | **0.083** | 0.072 | 0.067 | 0.065 | 0.073 | 0.077 | 0.069 | 0.057 | N / A | 0.071 |
| 29-JUN-2002 | 11 | 0.067 | 0.074 | 0.078 | 0.072 | 0.076 | 0.066 | 0.070 | 0.066 | **0.089** | 0.079 | 0.069 | 0.067 | N / A | 0.079 |
| 30-JUN-2002 | 11 | 0.067 | 0.074 | 0.080 | 0.071 | 0.078 | 0.074 | 0.070 | 0.069 | 0.088 | 0.080 | **0.093** | 0.074 | N / A | 0.068 |
| 01-JUL-2002 | 11 | 0.068 | 0.086 | 0.071 | 0.077 | **0.094** | 0.072 | 0.073 | 0.075 | 0.088 | 0.091 | 0.085 | 0.070 | N / A | 0.082 |
| 07-JUL-2002 | 9 | 0.062 | 0.067 | 0.070 | 0.067 | 0.071 | 0.059 | 0.066 | 0.060 | **0.081** | 0.076 | 0.069 | 0.072 | N / A | 0.080 |
| 09-JUL-2002 | 10 | 0.062 | 0.070 | 0.064 | 0.065 | **0.081** | 0.058 | 0.066 | 0.060 | 0.078 | 0.078 | 0.081 | 0.061 | N / A | 0.056 |
| 15-JUL-2002 | 11 | 0.062 | 0.065 | 0.070 | 0.064 | 0.068 | 0.058 | 0.066 | 0.058 | 0.076 | 0.074 | **0.085** | 0.055 | N / A | 0.063 |
| 18-JUL-2002 | 14 | 0.063 | 0.071 | 0.073 | 0.069 | 0.072 | 0.061 | 0.067 | 0.060 | 0.078 | 0.081 | **0.087** | N / A | N / A | 0.069 |
| 19-JUL-2002 | 10 | 0.074 | 0.086 | 0.086 | 0.083 | 0.089 | 0.067 | 0.084 | 0.070 | **0.092** | 0.091 | 0.092 | N / A | N / A | 0.069 |
| 20-JUL-2002 | 10 | 0.071 | 0.076 | 0.076 | 0.082 | 0.083 | 0.066 | 0.081 | 0.072 | 0.081 | **0.092** | 0.080 | N / A | N / A | 0.072 |
| 21-JUL-2002 | 10 | 0.065 | 0.076 | 0.066 | 0.070 | **0.080** | 0.061 | 0.071 | 0.066 | 0.073 | 0.078 | 0.069 | N / A | N / A | 0.067 |
| 10-AUG-2002 | 13 | 0.062 | 0.068 | 0.070 | 0.066 | 0.070 | 0.065 | 0.064 | 0.051 | **0.082** | 0.075 | 0.076 | 0.071 | N / A | 0.073 |
| 25-AUG-2002 | 14 | 0.060 | 0.063 | 0.064 | 0.063 | 0.064 | 0.057 | 0.059 | 0.046 | 0.073 | 0.071 | **0.080** | 0.064 | N / A | 0.066 |
| | | | | | | | | | | | | | | | |
| Max | 14.000 | 0.081 | 0.086 | 0.086 | 0.083 | 0.094 | 0.081 | 0.084 | 0.080 | 0.092 | 0.092 | 0.093 | 0.082 | 0.084 | 0.082 |

**Table 3-6.** Episode (July 18-21, 2002) average maximum 8-hour ozone concentrations versus average of fourth highest concentration from 2000-2002. (Source: CDPHE, 2003).

| Monitor | Episode Average Concentration (ppb) | Average of Fourth Highest Concentration from 2000-2002 (ppb) |
|---|---|---|
| NREL | 86 | 82 |
| Rocky Flats North | 81 | 84 |
| South Boulder Cr. | 75 | 74 |
| Highlands | 77 | 76 |
| Chatfield | 81 | 80 |

**Table 3-7.** Episode (June 25-July 1, 2002) average maximum 8-hour ozone concentrations versus average of fourth highest concentration from 2000-2002. (Source: CDPHE, 2003).

| Monitor | Episode Average Concentration (ppb) | Average of Fourth Highest Concentration from 2000-2002 (ppb) |
|---|---|---|
| NREL | 79 | 82 |
| Rocky Flats North | 84 | 84 |
| South Boulder Cr. | 73 | 74 |
| Highlands | 73 | 76 |
| Chatfield | 78 | 80 |

**Table 3-8.** Episode (June 8 – 12, 2002) average maximum 8-hour ozone concentrations versus average of fourth highest concentration from 2000-2002. (CDPHE, 2003).

| Monitor | Episode Average Concentration (ppb) | Average of Fourth Highest Concentration from 2000-2002 (ppb) |
|---|---|---|
| NREL | 71 | 82 |
| Rocky Flats North | 82 | 84 |
| South Boulder Cr. | 70 | 74 |
| Highlands | 64 | 76 |
| Chatfield | 64 | 80 |

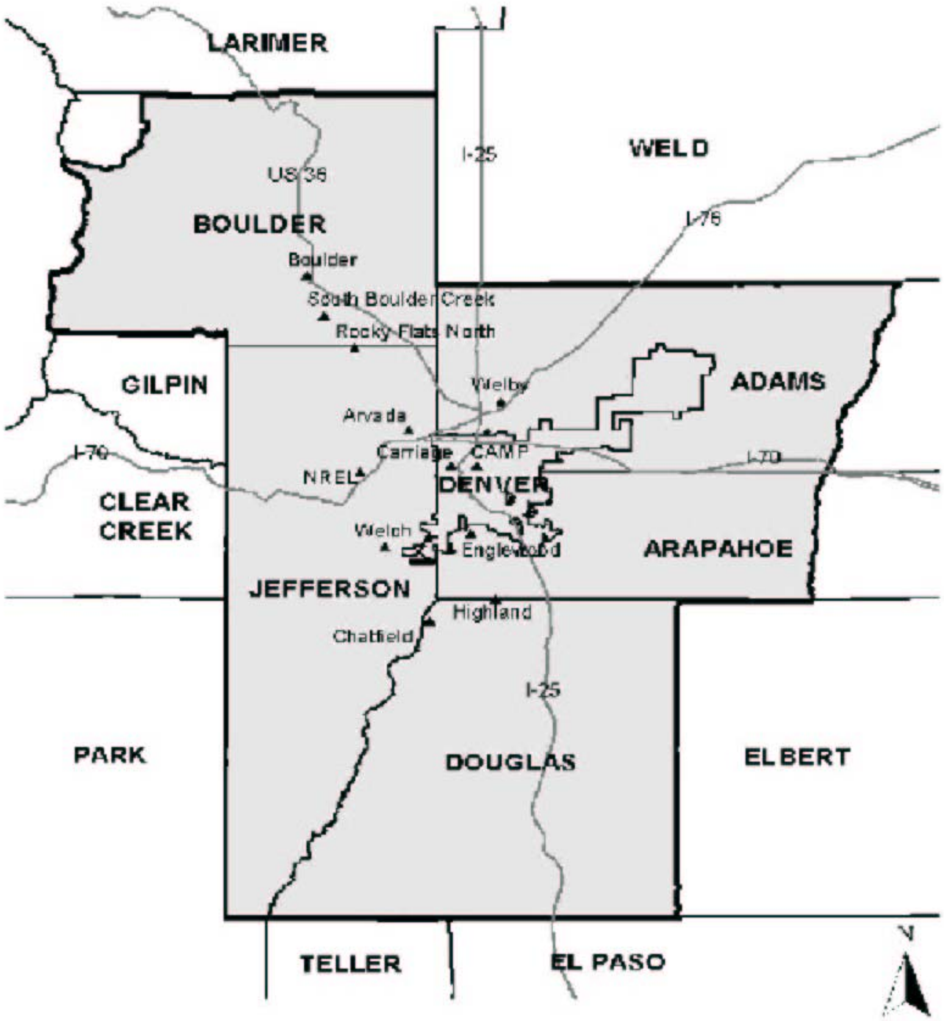



**Figure 3-1.** Map of the Denver Metropolitan one-hour ozone attainment/maintenance area and monitoring locations (Source: CDPHE, 2003).

# 4.0 MODELING DOMAINS AND DATA AVAILABILITY

## 4.1 Modeling Domains

This section identifies the modeling domains and grid specifications of the models to be used in the Denver 8-hr Early Action Compact Study. The recommended emissions, meteorological and photochemical modeling domains are consistent with the draft EPA 8-hr ozone modeling guidance wherever possible. Figure 4-1 through 4-4 and Table 4-1 present the spatial definitions of the emissions, photochemical and meteorological modeling domains. Below, we provide the summarize rationale underlying these domain selections.

### 4.1.1 Domains for Emissions and Air Quality Modeling

It is highly desirable to define the emissions and air quality modeling grids to match as closely as possible the meteorological grid configuration to minimize any interpolation processes which may distort the meteorological variables and introduce spurious effects (e.g., incorrect vertical velocities). It is also important to extend the air quality modeling domain as far as possible upwind to include all emission sources which have the potential to contribute substantially to elevated ozone concentrations in the Denver-Northern Front Range Region and to extend far enough downwind to address transport issues.

The emissions and air quality modeling domains are defined on an MM5 Lambert Conformal Projection (LCP) system as shown in Figure 4-1. This figure displays the LCP 36/12/4/1.33 km nested-grid structure to be used in the CAMx and EPS2x air quality and emissions modeling during the intensive episode periods. The CAMx nested modeling domains, shown in Figure 4-1 and defined in Table 4-1, are typically larger than most regulatory applications of ozone models. We selected the larger CAMx 36-km domain because of the reduction in the impact of boundary condition uncertainties on the ozone predictions that the larger domain affords. This is may be particularly important for 8-hr ozone since the typical concentrations are closer to the naturally occurring hourly background concentrations (40-60 ppb). The CPDHE episode selection analysis notes that there may be transport from Southern California and Texas during some periods. Thus, the high emission regions of the Los Angeles and Houston areas are included in the 36-km grid. The 12 km resolution domain covers the central Rocky Mountain states. The 36/12-km domains represent no computational difficulty on modern Linux computer clusters and will be operated for the entire June 7 through July 22, 2002 46 day period. More important however, from the standpoints of ozone prediction accuracy and computational requirements, is the finest grid resolution that will be needed. For the periods encompassing the two primary ozone episodes chosen for study (i.e., June 25-July 1, 2002 and July 18-21, 2002), we will invoke inner nests of 4 km and 1.33 km resolution to provide finer resolution of the emissions, transport, transformation, and removal processes. The 4-km grid will be initiated one day ahead of the two primary episodes to obtain fine scale initialization fields for the episode modeling. The June 8-12, 2002 secondary episode will be exercised with just the 4-km grid.

The CAMx 12-km resolution regional-scale domain will include the major source regions in the intermountain west (e.g., Salt Lake City, Phoenix, Houston, Albuquerque, Denver, Cheyenne, etc.) and extends as far north as Idaho. The 12-km domain will include most if not all of the states of Arizona, New Mexico, Colorado, Utah and large portions of Wyoming. The 4-km grid will be used for comparing CAMx model evaluation statistics with EPA's performance goals and for reporting the specific air quality metrics associated with the attainment demonstration (see Chapter 9). A 1.33 km high resolution domain ("Hi-Res Grid"), located over the Denver-Northern Front Range Region and including the Denver and Boulder metropolitan areas, will be used to corroborate the model source-receptor results on the nominal 4 km domain and to provide additional insight into the potential need for fine grid resolution in the DNFRR study area.

As indicated in Figure 4-5, in the vertical, a total of twenty-one (21) layers for the CAMx model will be used. The CAMx layer structure will be identical to the MM5 layer definitions in the first seventeen (17) levels to minimize any distortion of the meteorological variables. The number of layers in CAMx represents a substantial increase over that typically used in regulatory applications of photochemical models. However, we have found in past studies that this increased resolution provides better resolution for capturing the height of the daytime convective boundary layer (CBL), wind shear layers (significant for transport of pollutants aloft), and terrain-induced effects such as drainage flows, blocking and channeling. Early in the study we will evaluate the need for this many layers through sensitivity analysis and may reduce the number of vertical layers based on the balance between a desire for higher resolution versus pragmatic concerns about project schedule.

### 4.1.2 Meteorological Modeling Domain

Figures 4-2 and 4-3 present the nested MM5 domains at four levels of nesting: 36/12/4/1.33 km horizontal resolutions. In this DNFRR application, the 1.33 km 'Hi-Res' domain (Figure 4-3b) is located over the Denver-Boulder metropolitan area. For the MM5 modeling, the outer 36 km grid domain covers the entire continental U.S. and large portions of Canada and Mexico. This region is consistent with the recent continental scale, annual MM5 modeling Alpine has performed for the U.S. EPA and EPA Region 8 (see, for example, McNally and Tesche, 2002; 2003).

By using four nested grids at these resolutions (3:1 ratios), the needs of synoptic-scale accuracy, fine resolution, and consistency with the requirements of regional photochemical models is achieved. In addition, the meteorological modeling domain is configured so that: (1) the MM5 grids will align properly with the CAMx air quality grids, with some overlap; (2) additional 4-km and 1.33 km fine nests will be established to cover the Denver-Northern Front Range focus area, and (3) the MM5 LCP grid will be defined to be centered over the intermountain west domain. The horizontal resolution of the four MM5 nests are listed in Table 4-1. In the vertical, thirty four (34) layers for MM5 will be used. The vertical grid structure in MM5 is presented in Table 4-2. This grid layering is expected to provide adequate vertical resolution over the study region.

## 4.2 Data Availability

### 4.2.1 Emissions Data

Annual county-level area source emissions data, included off-road sources, will be provided by the CDPHE for the State of Colorado. Point source emissions are available from the CDPHE as well and will be provided by location, including appropriate stack parameters (stack height, stack diameter, exit temperature and exit velocity). On-road mobile sources will be provided to the Project Team in the form of link-based emissions from MOBILE6 within the urbanized areas of Denver, Greeley and Fort Collins. Beyond these urbanized areas, on-road mobile source emissions data will be provided at the county level. Pollutants to be provided include oxides of nitrogen (NOx), volatile organic compounds (VOC), carbon monoxide (CO), and sulfur dioxide (SO2). For regions of the air quality modeling domain outside Colorado, county-level emissions data will be obtained from the EPA's National Emission Inventory (NEI).

The CDPHE emissions inventory includes all major source categories including (a) stationary point sources, (b) area sources, (c) on-road mobile sources, and (d) off-road mobile sources. As described in section 5, these estimates will be developed for the base year (i.e., the historical year when the ozone episode actually occurred), the future baseline year (2007) and possibly various future-year emissions control scenarios and 2012. Construction of base year and projection emission inventories for each of these source categories requires a separate modeling approach as described in section 5.

### 4.2.2 Air Quality Data

Aerometric data from the AIRS data base for the modeling episodes and will be used in the development of photochemical model inputs and in evaluating the model's performance.

### 4.2.3 Meteorological Data

The predominant types of meteorological data to be used in this study will be surface and upper air meteorological measurements reported by the National Weather Service (NWS), and large-scale (i.e., regional/global) analysis databases developed by the National Center for Environmental Prediction (NCEP). Both types of data are archived by, and currently available from, the National Center for Atmospheric Research (NCAR). Measurement data include surface and aloft wind speed, wind direction, temperature, moisture, and pressure. Hourly surface data are usually available from many Class I airports, i.e., larger-volume civil and military airports operating 24-hour per day. The standard set of upper air data are provided by rawinsonde soundings launched every 12 hours from numerous sites across the continent. The typical spacing of rawinsonde site is approximately 300 km.

Eta analysis databases include 3-hourly 40 km. resolution analysis fields of winds, temperature, moisture, and pressure. The analysis data will be combined as necessary with measurement data for the following purposes:

- Developing initial and boundary inputs to MM5;

> Developing nudging fields for the MM5 FDDA package; and

> Evaluating MM5 predictive performance over the central U.S., with particular focus on the central Florida region.

Figure 4-3 shows the locations of the NWS upper air meteorological sounding data available from NCAR archives. Although this figure doesn't depict all of the currently available upper air sites, it does give a good overview of the number of sounding locations and their spatial distribution across the eastern U.S.

### 4.2.4 Terrestrial Data

The MM5 requires inputs of gridded terrain elevation and landuse/landcover codes for each grid specified in a simulation. NCAR provides access to several global and continental-scale terrain elevation and landcover databases of varying resolution. For example, the 36-km grid will use 10 minute topographic information derived from the Geophysical Data Center global data set. The 12-km grid will use the 5 min (~9.25 km) Geophysical Data Center global data set. Even finer resolution databases are available from NCAR for limited areas of North America; these would be used for the finest 4 km and 1.33 km grid nests.

The only terrestrial data required by CAMx is gridded land cover to define the spatial variation in pollutant deposition. For the coarsest 36-km grid, the same NCAR landcover databases will be used. However, the U.S. Geological Survey (USGS) provides 200-m pixel resolution land cover data for 1:250,000 scale quadrangle maps covering most of the U.S. These finer scale digitized maps will be used to provide land cover inputs for the finer CAMx grids.

**Table 4-1.** Grid definitions for the Denver EAC 8-hr Ozone Modeling study.

| Model | Grid Cells East-West | Grid Cells North-South | Lambert Grid Origin (km)From Pole (-93,40) |
|---|---|---|---|
| **EPS2x/CAMx** | | | |
| **- 36 km Grid** | 74 | 56 | -2304, -1404 |
| **- 12 km Grid** | 107 | 107 | -1560, -912 |
| **- 4 km Grid** | 146 | 122 | -1076, -292 |
| **- 1.33 km Grid** | 128 | 128 | -733.3, -73.3 |
| **MM5** | | | |
| **- 36 km Grid** | 165 | 129 | -2952, -2304 |
| **- 12 km Grid** | 127 | 127 | -1656, -1008 |
| **- 4 km Grid** | 163 | 151 | -1116, -372 |
| **- 1.33 km Grid** | 151 | 151 | -748.6, -88.6 |

**Table 4-2.** MM5 vertical grid structure.

| k(MM5) | sigma | press.(mb) | height(m) | depth(m) |
|---|---|---|---|---|
| 34 | 0.000 | 10000 | 15674 | 2004 |
| 33 | 0.050 | 14500 | 13670 | 1585 |
| 32 | 0.100 | 19000 | 12085 | 1321 |
| 31 | 0.150 | 23500 | 10764 | 1139 |
| 30 | 0.200 | 28000 | 9625 | 1004 |
| 29 | 0.250 | 32500 | 8621 | 900 |
| 28 | 0.300 | 37000 | 7720 | 817 |
| 27 | 0.350 | 41500 | 6903 | 750 |
| 26 | 0.400 | 46000 | 6153 | 693 |
| 25 | 0.450 | 50500 | 5461 | 645 |
| 24 | 0.500 | 55000 | 4816 | 604 |
| 23 | 0.550 | 59500 | 4212 | 568 |
| 22 | 0.600 | 64000 | 3644 | 536 |
| 21 | 0.650 | 68500 | 3108 | 508 |
| 20 | 0.700 | 73000 | 2600 | 388 |
| 19 | 0.740 | 76600 | 2212 | 282 |
| 18 | 0.770 | 79300 | 1930 | 274 |
| 17 | 0.800 | 82000 | 1657 | 178 |
| 16 | 0.820 | 83800 | 1478 | 175 |
| 15 | 0.840 | 85600 | 1303 | 172 |
| 14 | 0.860 | 87400 | 1130 | 169 |
| 13 | 0.880 | 89200 | 961 | 167 |
| 12 | 0.900 | 91000 | 794 | 82 |
| 11 | 0.910 | 91900 | 712 | 82 |
| 10 | 0.920 | 92800 | 631 | 81 |
| 9 | 0.930 | 93700 | 550 | 80 |
| 8 | 0.940 | 94600 | 469 | 80 |
| 7 | 0.950 | 95500 | 389 | 79 |
| 6 | 0.960 | 96400 | 310 | 78 |
| 5 | 0.970 | 97300 | 232 | 78 |
| 4 | 0.980 | 98200 | 154 | 39 |
| 3 | 0.985 | 98650 | 115 | 39 |
| 2 | 0.990 | 99100 | 77 | 38 |
| 1 | 0.995 | 99550 | 38 | 38 |
| 0 | 1.000 | 100000 | 0 | 0 |

**Table 4-3.** Comparison of MM5 and CAMx vertical grid structures. (The CAMx 36/12/4/1.33 km grids will all initially contain 21 vertical layers, vertical layer sensitivity tests will be conducted to determine the optimal number of vertical layers).

| MM5 Layer K | Interface Heights Height (m) | CAMx Layer Interface Heights |
|---|---|---|
| **28** | 6521 | 21 |
| **25** | 4660 | 20 |
| **22** | 3132 | 19 |
| **19** | 1911 | 18 |
| **17** | 1434 | 17 |
| **16** | 1280 | 16 |
| **15** | 1129 | 15 |
| **14** | 981 | 14 |
| **13** | 834 | 13 |
| **12** | 690 | 12 |
| **11** | 619 | 11 |
| **10** | 548 | 10 |
| **9** | 478 | 9 |
| **8** | 409 | 8 |
| **7** | 340 | 7 |
| **6** | 271 | 6 |
| **5** | 203 | 5 |
| **4** | 135 | 4 |
| **3** | 102 | 3 |
| **2** | 68 | 2 |
| **1** | 35 | 1 |

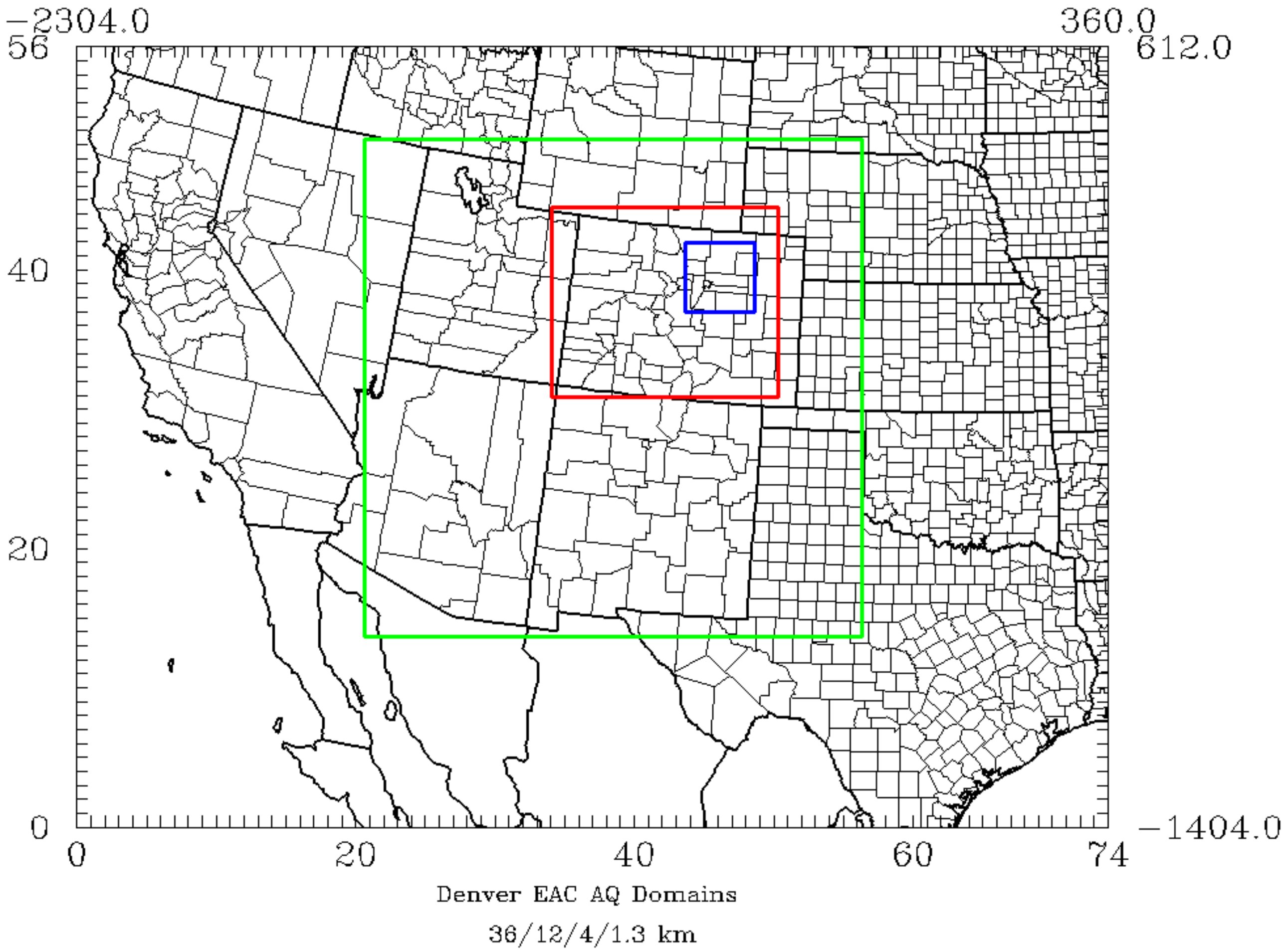



**Figure 4-1.** Proposed nested 36/12/4/1.33-km emissions and photochemical modeling domain for the Denver EAC 8-hr Ozone study. (Outer grid has 36 km horizontal spacing; green grid is the 12 km domain; red grid is the 4 km domain; the blue grid is the 1.33 km "Hi-Res" domain over the greater Denver metropolitan area.)

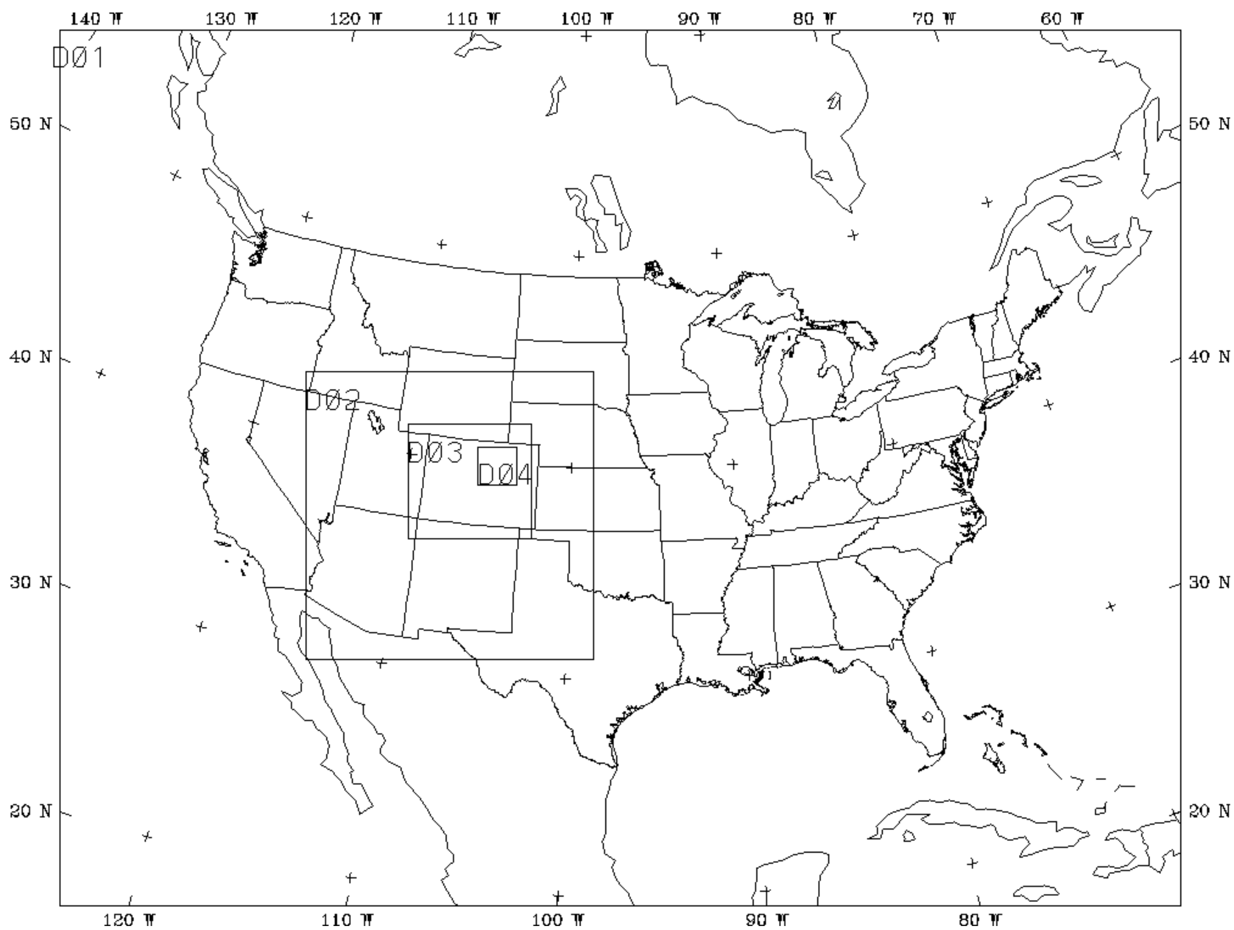
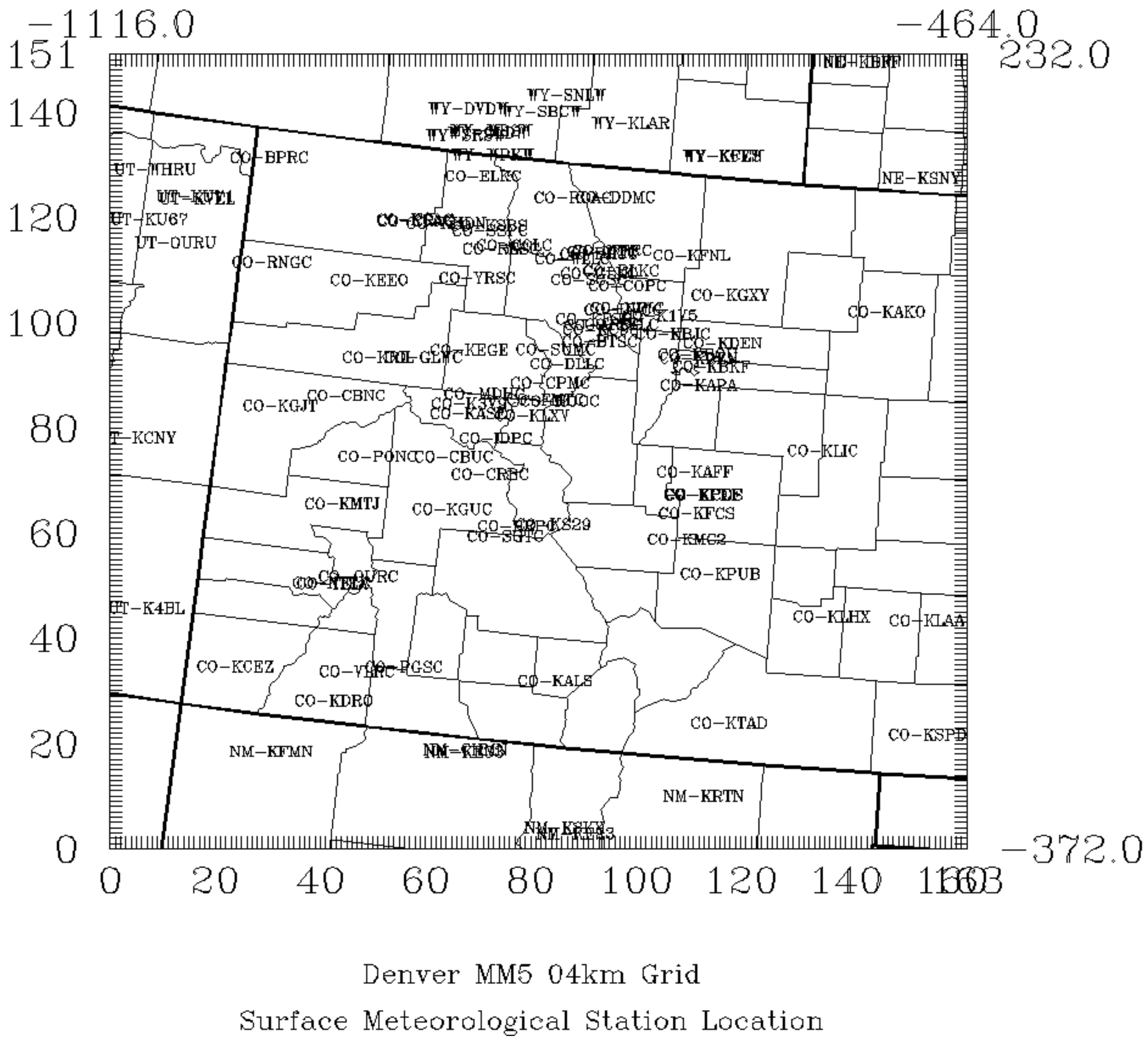
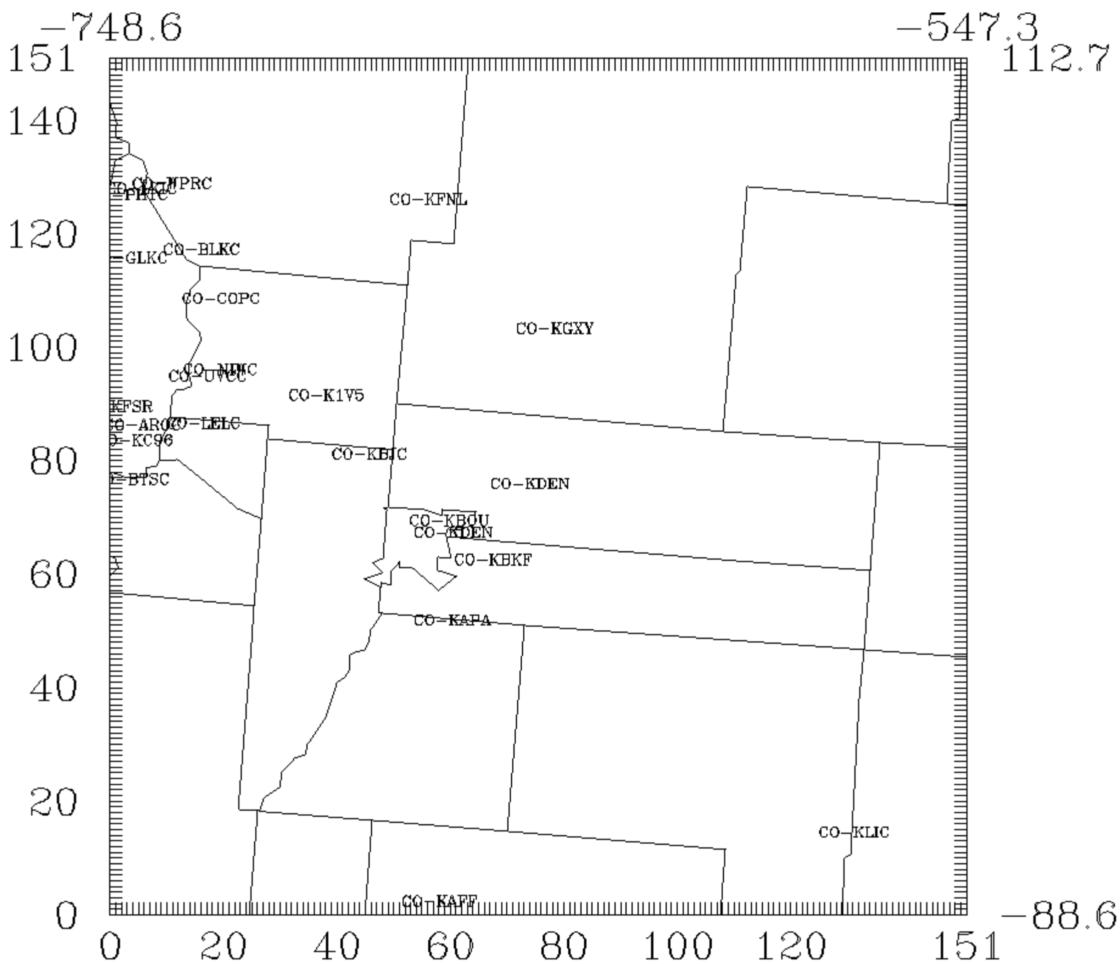



**Figure 4-2.** Proposed nested 36/12/4/1.33-km meteorological modeling domain for the Denver EAC 8-Hr Ozone study.




(a) 4 km Grid Domain

**Figure 4-3.** Location of nested MM5 grids and air quality monitoring stations for the Denver EAC 8-Hr Ozone study.




Denver MM5 1.3 km Grid

Surface Meteorological Station Location

(b) 1.33 km Grid Domain

**Figure 4-3.** Continued.

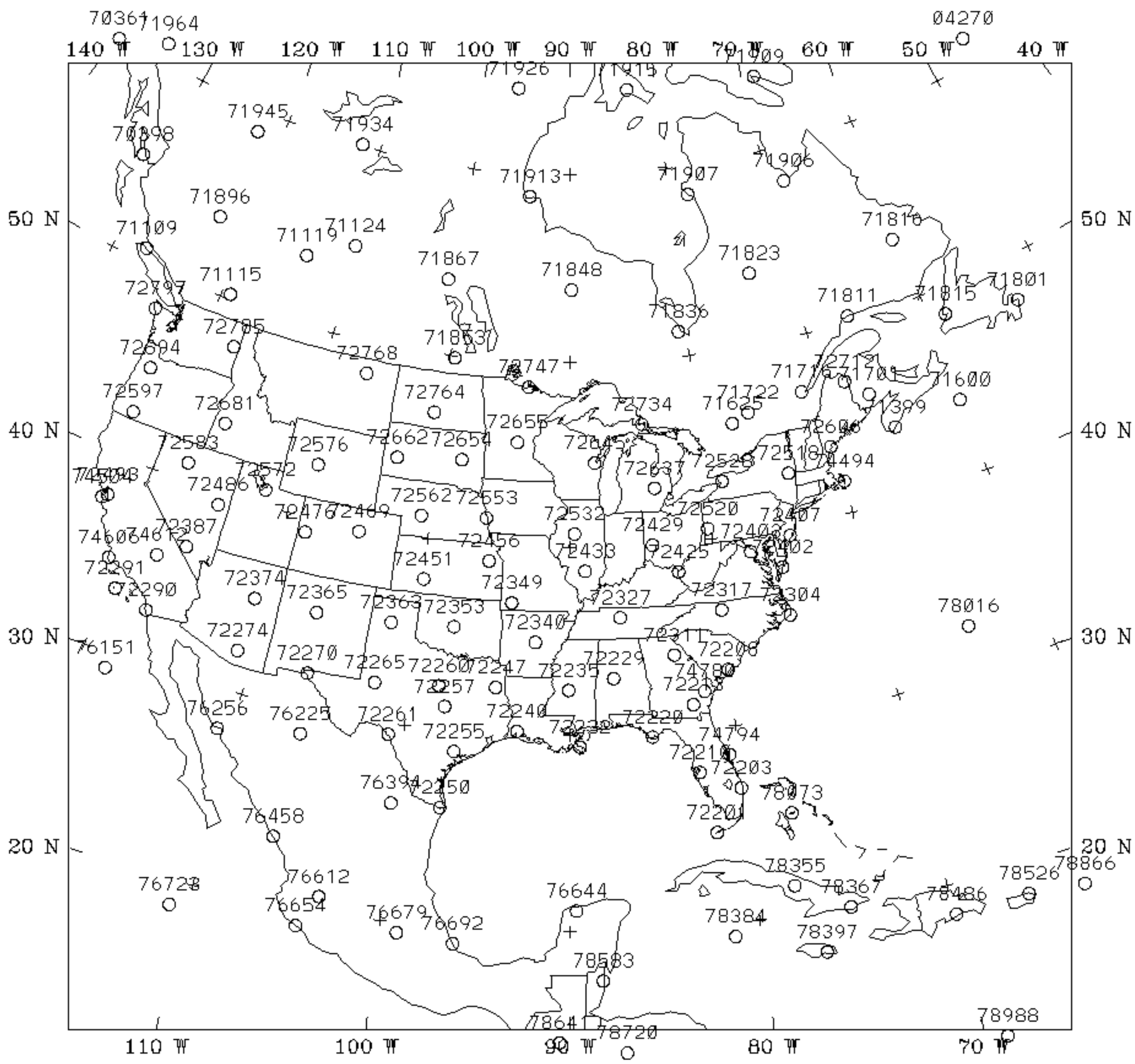



**Figure 4-4.** Location of upper air sounding sites throughout the U.S. to be used in the MM5 prognostic meteorological modeling for the Denver EAC 8-hr Ozone study.

# 5.0 INPUT DATA PREPARATION PROCEDURES

This section describes how the emissions, meteorological and air quality modeling data sets will be developed for the Denver EAC 8-hr Ozone Study using the EPS2x, MM5, and CAMx modeling software. Additional details describing the model algorithms and modeling procedures are contained in the literature citations.

## 5.1 Development Of Base Year And Future Year Emissions Inventories For Photochemical Modeling

In this study, county-wide base year emissions inventories will be developed and supplied to the ENVIRON/Alpine team by CDPHE. These data sets will then be used as input to the EPS2x model to apply temporal, spatial, and chemical speciation factors as well as adjustments to the mobile source emissions for the specific pressure and temperature conditions during the two primary episode intensive periods of the Summer '02 modeling episode. This effort will produce the model-ready base-year inventories and the opportunity to conduct additional quality assurance (QA) of the emissions data sets.

### 5.1.1 Base Case Emissions Inventory Processing

The Countywide emissions will be provided by the CDPHE, for the state of Colorado and will be augmented by emissions from the NEI99 inventory for the other states. This information will be processed with EPS2x to generate the gridded speciated hourly emissions inputs required by the CAMx photochemical grid model. The first step in the emissions processing will be a quality assurance of the emissions data provided by the CPDHE and supplemental data from the NEI99. Link-based on-road mobile source emissions will be provided by CDPHE for the Denver region for use in generating the on-road mobile source emissions.

Surrogate distributions of land use categories, population, etc. will be generated using GIS techniques at four grid resolutions: 36 km, 12 km; 4 km; and 1.33 km. The county-level emissions provided by the CDPHE for Colorado and the NEI data for outside Colorado will be spatially allocated to the grid using the surrogate distributions and then temporally allocated to day of week and then hour of day using either temporal allocation factors provided with the CDPHE emissions database or default profiles that are based on Source Industry Code (SIC) and Source Classification Code (SCC). The gridded hourly emissions would then be chemically speciated to the chemical species in the Carbon Bond IV (CB-IV) chemical mechanism using the standard default speciation profiles that are based on SIC/SCC codes.

One area that has not been included in emissions inventories in the past but will in this study is base year inventory will be the emissions from the large concentrations of oil and gas wells in Weld County. As indicated in Figure 5-1, there are a substantial number of wells located over a productive coal seam east of the Front Range. Typically, oil and gas exploration and development activities produce unwanted quantities of gases that contain both $CO_2$ and VOCs. When these gases are released between field holding tanks and transfer trucks, so-called "flash emissions" may results. While natural gas wells do not produce these emissions, they are commonly released from oil wells. While individual "flash emission" transfer points produce fairly small emissions of VOCs per well, as indicated in Figure 5-1 there are about 2000 of these points in Weld County. Other areas such as La Plata County are not over the type of coal seams that produce "flash emissions".

The CPDHE will provide link-based MOBILE6 emissions for the greater Denver area that will be gridded and speciated to the 4/1.33 km modeling grid. Outside of the Denver area the CPDHE will provide county-level MOBILE6 emissions that will be gridded on the domains identified in Figure 4-1. Outside of Colorado, mobile sources emissions from the NEI99 will be used projected to the Summer ’02 episode. For the 36 and 12km grid domains, three gridded emissions inventory impacts will be prepared corresponding to a typical summer weekday, Saturday and Sunday. For the 4 and 1.33 km domains and during the episode periods, on-road mobile source emissions will be adjusted using the episode-specific temperatures from the MM5 simulation of this period. Area and off-road emissions provided by the CDPHE and augmented by the NEI99 inventory will be gridded, speciated, and temporally allocated to the pertinent gridded modeling domains discussed in section 4. Biogenic emissions will be generated using the GLoBEIS model and MM5 episodic specific temperature data.

During the Summer 02 modeling period there were numerous wildfires in the western US some of which affected air quality in the Denver area. These wild fires emit significant amounts of NOx, VOC and CO that are precursors to ozone formation. Furthermore, the smoke from the fires affect incoming ultraviolet radiation so alter photolysis rates. The development of an emission inventory for fires is a time consuming task. The Western Regional Air Partnership (WRAP) is embarking on a study to develop a fire emissions inventory for major fires in 2002 that is expected to be available by the end of 2003, which is too late for the Denver EAC modeling. Thus, the initial Denver EAC modeling will not include emissions from fires. If preliminary emissions from wildfires for the episode period become available then they will be included in the analysis. As emissions from wildfires are highly uncertain, bounding sensitivity tests will be performed to determine whether they had the potential to contribute to the elevated 8-hour concentrations.

An important component of the emissions modeling will be quality assurance and quality control (QA/QC). EPS2x will be used to make internal QA/QC checks of the emissions data sets. These consistency checks will be performed to verify that the mass of emissions entering and leaving each major emissions processing step (e.g., temporal allocation, gridding, and speciation) from the raw data provided by the CDPHE to the model-ready gridded hourly speciated inventory are the same and any lost emissions are attributable to a specific known reason (e.g., county being on the edge of the modeling domain). The results of the emissions modeling would be displayed in maps of spatial distributions of emissions and summary tables of emissions by subregions (e.g., counties and/or modeling domain grids).

### 5.1.2 Future Year Base Line Emissions Inventory Processing

Year 2007 countywide baseline emissions inventories will be obtained from the CDPHE and processed with the emissions modeling system to render them model-ready for CAMx. Essentially the same procedures used in the base case inventory processing will be used for the future year baseline emissions development. The typical information and data that are available to compile the 2007 inventory include (a) updated point and area source control information, (b) future year emissions estimates for large utility and industrial sources, (c) information on start-ups/shutdowns of large plants, (d) future-year VMT/MOBILE 6.2 inputs, and appropriate growth factors (e.g., BEA). In addition to processing the CDPHE's 2007 baseline inventory, we will carryout an independent statistical and graphical QA analysis to confirm the soundness and reasonableness of the emissions files.

## 5.2 Meteorological Inputs And Mm5 Modeling

The databases and modeling procedures to be used to set up, exercise, and evaluate the MM5 model for the Summer '02 episode are summarized in this section.

### 5.2.1 Fixed Inputs

Topography Topographic information will be developed using the National Center for Atmospheric Research (NCAR) terrain databases. The 36 km and 12km grids will use 5 min topographic information derived from the Geophysical Data Center global data set while the 4 km and 1.33 km grids will use the 30 sec resolution data set. Terrain data will be interpolated to the model grids using a Cressman-type objective analysis scheme.

Vegetation Type and Land Use: Vegetation type and land use information will be developed using the NCAR/PSU 10 min. (~18.5 km) databases for the 36 km grid and from the United States Geological Survey (USGS) data for the 12 km ,4 km and 1.33 km grids. Surface characteristics correspond to each land use category in the MM5 modeling domain will be consistent with those used CAMx and are discussed in McNally and Tesche (2002, 2003).

### 5.2.2 Variable Data Inputs

Atmospheric Data: Initial conditions to the MM5 will be developed from operationally analyzed fields derived from the National Center for Environmental Predictions (NCEP) ETA (40 km resolution) following the procedures outlined by Stauffer and Seaman (1990). The synoptic-scale data to be used in the initialization (and in the analysis nudging discussed below) will be obtained from the conventional National Weather Service (NWS) twice-daily radiosondes and standard 3-hr NWS surface observations. These data include the horizontal wind components (u and v), temperature (T), and relative humidity (RH) at the standard pressure levels, plus sea-level pressure (SLP) and ground temperature ($T_g$). Here, $T_g$ represents surface temperature over land and sea-surface temperature over water.

The so-called "first guess" NMC-analyzed fields will be interpolated to several supplemental analysis levels (e.g., 950, 900, 800, and 600 mb) and then modified by blending in the NWS standard rawinsonde data using a successive-correlation type of objective analysis that accounts for enhanced along-wind correlation of variables in strongly curved flow (Benjamin and Seaman, 1985). Subsequently, the three-dimensional variable fields will be interpolated onto the MM5's sigma vertical coordinate system. On the 36 km grid (Grid D01), the analyses will be performed using a Cressman-type procedure and then interpolated to the 12 km, 4 km and 1.33 km grids (Grids D02, D03, and D04) in Figure 4-2.

Lateral boundary conditions to the MM5 will be specified from observations by temporally interpolating the 12-hourly enhanced analyses described above. The inner meshes will be operated in a two-way interactive mode with the next outer grids and received their boundary conditions at one-hour intervals. For each time step between the times for which new boundary conditions were available, a temporal interpolation is performed to provide smoothly changing boundary values to the appropriate nested meshes.

Water Temperature: Water temperatures will be derived from the ETA skin temperature variable. These temperatures are then bi-linearly interpolated to each model domain and, where necessary, filtered to smooth out irregularities.

Clouds and Precipitation: While the non-hydrostatic MM5 treats cloud formation and precipitation directly through explicit resolved-scale and parameterized sub-grid scale processes, the model does not require precipitation or cloud input. The potential for precipitation and cloud formation enters through the thermodynamic and cloud processes formulations in the model. The only precipitation-related input required is the initial mixing ratio field that is developed from the NWS and NMC data sets previously discussed.

### 5.2.3 Multi-Scale FDDA

The multi-scale Four Dimensional Data Assimilation (FDDA) technique developed at Penn State (Stauffer and Seaman, 1990, 1994; Stauffer et al., 1985, 1991) is based on Newtonian relaxation, or nudging, which is a continuous assimilation method that relaxes the model state toward the observed state by adding to one or more of the prognostic equations artificial tendency terms based on the difference between the two states. It is basically a form of continuous data assimilation because the nudging term is applied at every time step, thereby minimizing "shock" to the model solutions that may occur in intermittent assimilation schemes. The standard FDDA methodology includes two options: (a) nudging toward gridded analyses which are interpolated to the model's current time step, and (b) nudging directly toward individual observations within a time-and-space "window" surrounding the data. These two approaches are referred to as "analysis nudging" and "obs-nudging", respectively. Analysis nudging is ideal for assimilating synoptic data that cover most or all of a model domain at discrete times. Obs-nudging does not require gridded analyses of observations and is better suited for assimilating high-frequency asynoptic data that may be distributed non-uniformly in space and time (i.e., the Lake Michigan Ozone Study intensive studies data).

A “multi-scale” data assimilation strategy will be used with MM5 in this study. This methodology, developed by researchers at Penn State University (Shafran and Seaman, 1998) employs both FDDA methods. Standard “analysis nudging” will be used on the outer grids using objectively analyzed three-dimensional fields produced every 3-hr from the NWS rawinsonde wind, temperature, and mixing ratio data, and similar analyses generated every three hours from the available NWS surface data. More specifically, analysis nudging will only be used on the outer two grids (i.e., 36 km and 12 km) and the size of the nudging coefficient used for the assimilation of wind, temperature and moisture will be $2.5 \times 10^{-4}$ for winds and temperature and $1.0 \times 10^{-4}$ for mixing ratio.

### 5.2.4 Physics Options

The MM5 model physics options to be used in the present application are as follows.

Planetary Boundary Layer Schemes. The Pleim-Chang planetary boundary layer scheme will be used. This PBL scheme is a derivative of the Blackadar PBL scheme called the Asymetric Convective Model using a variation on Blackadars non-local mixings.

Explicit Moisture Schemes. Resolved-scale precipitation processes will be treated explicitly with a simple water/ice scheme (no supercooled water substance) following the approach of Dudhia (1989 For the 12 km and 36 km mesoscale grids, the Kain-Fritsch scheme will be used. This parameterization achieves closure via convective available potential energy and an entraining/detraining cloud model. Furthermore, it parameterizes moist convective downdrafts. No convective parameterization will be performed on the 4 km and 1.3km mesh since we will assume that convection is explicitly resolved at this scale.
Radiation Scheme. The Rapid Radiative Transfer Model (RRTM) longwave scheme will be used. The RRTM is a new highly accurate and efficient method.

Land Surface Model. The Pleim-Xiu (PX) land surface model will be used. This scheme represents soil moisture and temperature in two layers (surface layer at 1cm and root zone at 1m) as well as canopy moisture. It handles soil surface, canopy and evapotranspiration moisture fluxes. The PX scheme will be run in a continuous mode throughout the entire episode.

Grid Nesting: The 36km and 12km domains will be run with continuous updating without feedback from the finer grid to the coarser grid. The 4km domain will be run with hourly updating from the 12km domain. The 1.3km domain will be run with continuous updating of the 4km domain.

## 5.3 Photochemical Modeling Inputs

The databases and modeling procedures used to set up, exercise, and evaluate the CAMx (ver 4.0) model for the Summer '02 episode are summarized below. The CAMx model will be exercised with the CB-IV chemistry and the CMC chemistry solver. The PPM horizontal advection scheme has been selected due to its significant accuracy and we recommend employing CAMx's two-way interactive grid nesting option.

### 5.3.1 Meteorological Inputs

As noted, meteorological inputs to the CAMx model will be developed using the PSU/NCAR Mesoscale Meteorological Model (MM5). All of the essential meteorological fields required to exercise CAMx (e.g., three dimensional winds, temperatures, turbulence parameters, and so on) will be developed directly from the MM5 output fields. The 'MM5CAMx' processor will be used to map MM5 gridded output data to the parameters and formats required by CAMx. The program assumes that the horizontal grids between the two models match exactly, i.e., the CAMx physical-height layer structure is defined as a subset of the space-varying (time-invariant) MM5 sigma-p layers. CAMx also requires fields of cloud water, horizontal cloud coverage, and vertical extent in each model column and above the model. These fields will be produced in the MM5 and formatted by 'MM5CAMx' for input to CAMx.

### 5.3.2 Initial and Boundary Conditions

Boundary conditions represent pollution inflow into the model and initial conditions provide an estimation of pollution that already exists. The initial conditions are usually considered to be background concentrations of pollutants. Both initial and boundary conditions may vary in time and in vertical space. The impact of initial concentrations within the boundary layer is small over month-long episodes, but a larger impact may occur in the upper troposphere (Tonneson et al, 2001). The initial and boundary conditions to be used for the CAMx model on the outer 36 km grid (see Figure 4-1) will be consistent in the horizontal and vertical direction and based on representative Tropospheric profiles suggested by EPA with the June 2002 release of the CMAQ model and as modified by the Western Regional Air Partnership (WRAP) modeling. Where an initial or boundary concentration is not specified for a pollutant the model will default to a near-zero concentration.

### 5.3.3 Air Quality and Chemistry Inputs

The ozone observations to be used in the model evaluation will be taken from the U.S. EPA Airs AQS database. The chemical species, rate constants, and other parameters contained in the current regulatory version of the CBM-IV chemical mechanism (with the isoprene updates) will be used as input to the CAMx model.

### 5.3.4 Vegetation and Land Use

Vegetation type and land use information will be developed using a combination of the NCAR/PSU terrestrial database and the USGS high resolution (200 m pixel) landuse/landcover database. For all grids, the 300 m USGS CTG database will be used. Standard CAMx preprocessors will be employed to translate the USGS land cover codes to appropriate CAMx inputs.

### 5.3.5 Particulate Matter Inputs

CAMx version 4 is a one-atmosphere model that includes aerosol modules for treating particulate matter (PM) compounds. Involving the PM treatment in CAMx results in increases in computer run times to accommodate the additional species and computational requirements of the aerosol modules. However, simulating PM has very little feed back on the CAMx estimated ozone concentrations. Thus, for the Denver 8-hour ozone EAC application we will exercise the CAMx model without PM using the CAMx mechanism 3 option. However, we will prepare the emission and initial and boundary condition (IC/BC) inputs to accommodate the CAMx mechanism 4 PM treatment. In this way CAMx may be run in a one-atmosphere ozone and (PM mode in the future using the exact same inputs as used in the EAC ozone modeling.

**Table 5-1.** Description of land use categories and physical parameters.

| Land Use Integer Identification | Land Use Description | Albedo (%) | Moisture Avail. (%) | Emissivity (% at 9 micrometers) | Roughness Length (cm) | Thermal Inertia (cal cm-2 k-1 s-1/2) |
|---|---|---|---|---|---|---|
| 1 | Urban Land | 18 | 5 | 88 | 50 | 0.03 |
| 2 | Agriculture | 17 | 30 | 92 | 15 | 0.04 |
| 3 | Range-grassland | 19 | 15 | 92 | 12 | 0.03 |
| 4 | Deciduous Forest | 16 | 30 | 93 | 50 | 0.04 |
| 5 | Coniferous Forest | 12 | 30 | 95 | 50 | 0.04 |
| 6 | Mixed Forest and Wet Land | 14 | 35 | 95 | 40 | 0.05 |
| 7 | Water | 8 | 100 | 98 | 0.01 | 0.06 |
| 8 | Marsh or Wet Land | 14 | 50 | 95 | 20 | 0.06 |
| 9 | Desert | 25 | 2 | 85 | 10 | 0.02 |
| 10 | Tundra | 15 | 50 | 92 | 10 | 0.05 |
| 11 | Permanent Ice | 55 | 95 | 95 | 5 | 0.05 |
| 12 | Tropical or SubTropical Forest | 12 | 50 | 95 | 50 | 0.05 |
| 13 | Savannah | 20 | 15 | 92 | 15 | 0.03 |

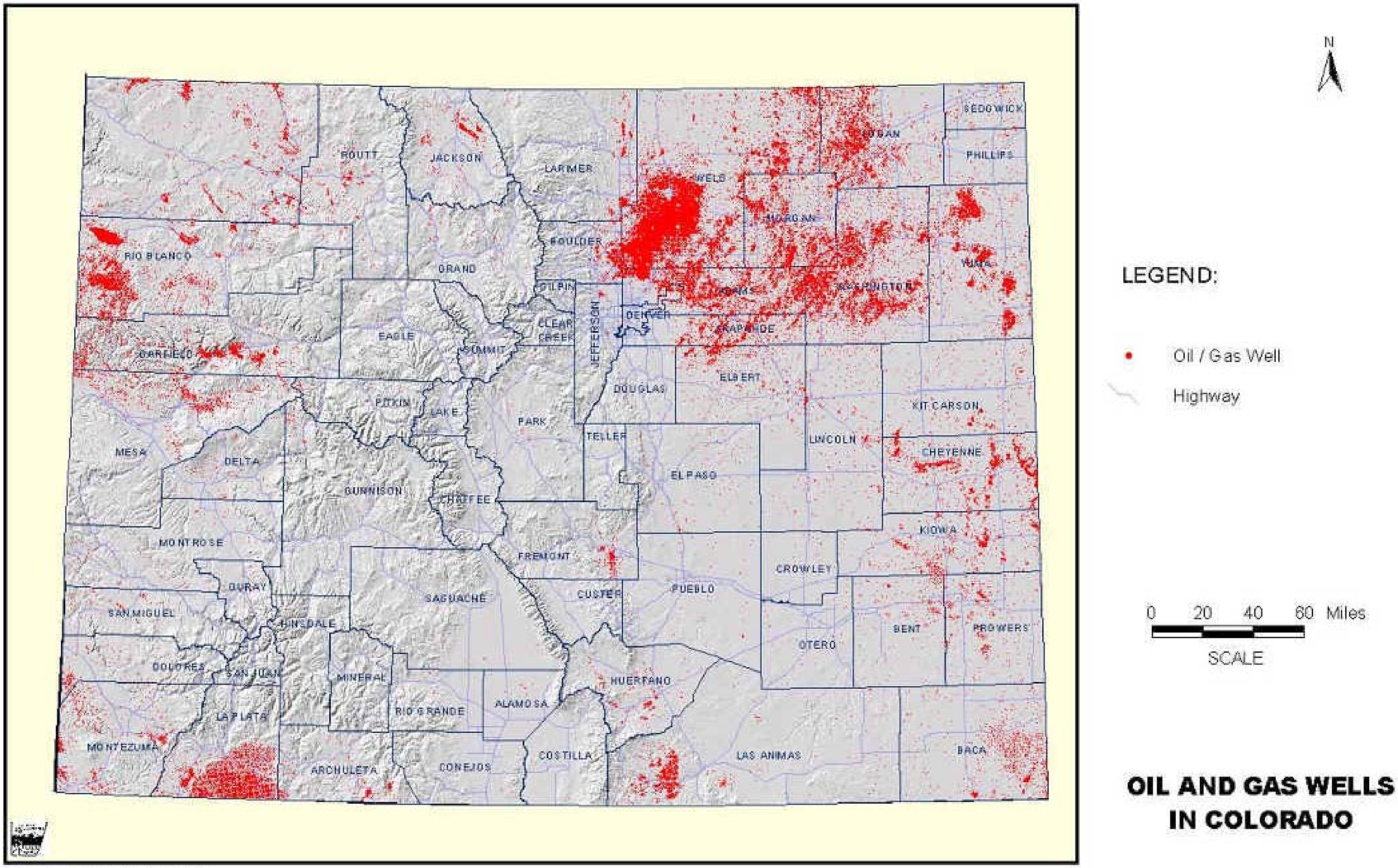



**Figure 5-1.** Location of flash emissions points from oil and gas wells in Colorado (source: CDPHE).

# 6.0 QUALITY ASSURANCE

Quality Assurance (QA) activities will be carried out for the various emissions, meteorological, and photochemical modeling components of the Denver EAC 8-hr ozone modeling study. Examples of the type of activities to be performed are given below.

## 6.1 Emissions Model Inputs And Outputs

The emissions inventories obtained from the CDPHE as well as from other organizations including the EPA, other governmental agencies, industry, and stakeholders will be examined principally through the use of the EPS2x quality assurance software, algorithms, and plotting routines. EPS2x produces various reports that allow the emissions modeler to check rapidly for gross errors in the emissions estimates. When such errors are discovered, the problems in the input data files are corrected and the EPS2x model rerun. Other more subtle errors are typically discovered during the post-EPS2x5 quality assurance phase. During a post-processing check, the emissions estimates are run through the MAPS and/or PAVE software programs (McNally and Tesche, 1994) or other display programs which produce graphical displays of the emissions estimates over the modeling domain and temporal graphs of the emissions estimates. These graphs may be examined for anomalous values (e.g. localized emissions over a lake, high emissions in a rural setting), and when discovered, the problems in the emission input files are diagnosed, corrected, and the EPS2x model rerun.

## 6.2 Meteorological And Photochemical Model Inputs And Outputs

The MM5 meteorological and CAMx air quality model inputs and outputs will be plotted and examined to ensure: (a) accurate representation of the observed data in the model-ready fields, and (b) temporal and spatial consistency and reasonableness. As noted in section 7, both MM5 and CAMx will undergo an operational/scientific evaluation and this will facilitate, among other things, the quality assurance review of the meteorological and air quality modeling procedures. Data sets available to support this quality assurance of the aerometric inputs include the routine synoptic-scale data sets from the NWS 12-hourly rawinsondes and 3-hourly surface observations. These data include the horizontal wind components (u and v), temperature (T), and relative humidity (RH) at the standard pressure levels, plus sea-level pressure (SLP) and ground temperature ($T_g$). i.e., the surface temperature over land and sea-surface temperature over water.

# 7.0 MODEL PERFORMANCE EVALUATION

Model performance evaluation (MPE) is the process of testing a model's ability to estimate accurately observed atmospheric properties over a range of synoptic and geophysical conditions. When conducted thoughtfully and thoroughly, the process focuses and directs the continuing cycle of model development, data collection, model testing, diagnostic analysis, refinement, and re-testing. In this section we summarize the philosophy and objectives that will govern the evaluation of the MM5 prognostic and CAMx photochemical models for the DNFRR application. We then identify the specific evaluation methods that will employed to judge the suitability of the MM5 and CAMx models for regulatory applications, using common statistical measures and graphical procedures to elucidate model performance. This evaluation plan conforms to the procedures recommended by the EPA (1991, 1999) for 1-hr and 8-hr ozone attainment demonstration modeling.

## 7.1 Principles

We begin by establishing a framework for assessing whether the MM5/CAMx modeling system (i.e., the emissions, meteorological and dispersion models and their supporting data sets) performs with sufficient reliability to justify its use in developing ozone control strategies. The model's reliability will be assessed given consideration to the following principals:

> **The Model Should be Viewed as a System.** When we refer to evaluating a "model", we mean this in the broad sense. This includes not only the CAMx photochemical model, but its various components: companion preprocessor models (i.e., the EPS2x emissions and the MM5 meteorological models), the supporting aerometric and emissions data base, and any other related analytical and numerical procedures used to produce modeling results. A principal emphasis in the model testing process is to identify and correct flawed model components;

> **Model Acceptance is a Continuing Process of Non-Rejection.** Over-reliance on explicit or implied model "acceptance" criteria should be avoided. This includes EPA's so-called performance goals (EPA, 1991). Models should be accepted gradually as a consequence of successive non-rejections. Over time, confidence in a model builds as it is exercised in a number of different applications (hopefully involving stressful performance testing) without encountering major or fatal flaws that cause the model to be rejected;

> **Criteria for Judging Model Performance Must Remain Flexible.** The criteria for judging the acceptability of model performance should remain flexible, recognizing the challenging requirement of the DNFRR application including the use of : (a) a nested regional model (CAMx), (b) new emissions data sets developed by the CDPHE, and (c) prognostic model output (MM5) at physical scales as fine as 1.33 km; and

> **Previous Experience Used as a Guide.** Previous photochemical modeling experience serves as a primary guide for judging model acceptability. Interpretation

of the CAMx modeling results for each episode, against the backdrop of previous modeling experience, will aid in identifying potential performance problems and suggest whether the model should be tested further or rejected.

These principals have been incorporated into the following operational methodology for testing the performance of the MM5/CAMx modeling system for both 1-hr and 8-hr ozone concentrations as recommended in the EPA guidelines.

## 7.2 Meteorological Model Evaluation Process

Meteorological inputs required by CAMx include hourly estimates of surface pressure and clouds; the three-dimensional distribution of winds, temperatures, and mixing ratio; and other physical parameters or diagnosed quantities such as turbulent mixing rates (i.e., eddy diffusivities) and planetary boundary layer heights. Accordingly, the objective of the MM5 performance evaluation is to assess the adequacy of these surface and aloft meteorological fields. More specifically, we seek to assess the adequacy and reliability of the dynamic and thermodynamic meteorological fields for input to the CAMx regional photochemical model. The MM5 evaluation will be founded upon comparisons between hourly modeled predictions and surface and aloft meteorological measurements obtained principally from National Weather Service (NWS) sites and at various air monitoring stations.

### 7.2.1 Components of the MM5 Evaluation

The MM5 modeling system is well-established with a rich development and refinement history spanning more than two decades (Seaman, 2000). The model has seen extensive use worldwide by many agencies, consultants, university scientists and research groups. Thus, the current version of the model as well as its predecessor versions have been extensively "peer-reviewed" and considerable algorithm development and module testing has been carried out with all of the important process components. Given that the MM5 model code and algorithms have already undergone significant peer review, performance testing of the MM5 model in this study will be focused on an operational evaluation.

The *operational evaluation* refers to an assessment of a model's ability to estimate atmospheric observations independent of whether the actual process descriptions in the model are accurate (Tesche, 1991a,b). It is an examination of how well the model reproduces the observed meteorological fields in time and space consistent with the input needs of the air quality model. Here, the primary emphasis is on the model's ability to reproduce hourly surface wind speed, wind direction, temperature, and mixing ratio observations across the 12/4/1.33 km grid domains. The operational evaluation provides very useful information but is somewhat limited in revealing whether the results are correct from a scientific perspective or whether they are the fortuitous product of compensating errors.

A "successful" operational evaluation is a necessary but insufficient condition for achieving a sound, reliable performance testing exercise. An additional scientific evaluation is also needed. The *scientific evaluation* attempts to elucidate the realism of the basic meteorological processes simulated by the model. This involves testing the model as an entire system (i.e., not merely focusing on surface wind predictions) as well as its component parts. The scientific evaluation seeks to determine whether the model's behavior in the aggregate and in its component modules is consistent with prevailing theory, knowledge of physical processes, and observations. The main objective is to reveal the presence of bias and internal (compensating) errors in the model that, unless discovered and rectified, or at least quantified, may lead to erroneous or fundamentally incorrect technical or policy decisions. Typically, the scope of the scientific evaluation is limited by the availability of special meteorological observations (radar profiler winds, turbulence measurements, PBL heights, precipitation and radiation measurements, inert tracer diffusion experiments, and so on). Unfortunately, since none of these measurements are available over the Denver region during the summer of 2002, a meaningful scientific evaluation of the MM5 is not possible in this study. However, we believe the operational evaluation will be quite sufficient to determine whether the model is operating with sufficient reliability to be used in the photochemical modeling portion of the study.

### 7.2.2 Data Supporting Model Evaluation

Hourly surface observations will be obtained from the National Center for Atmospheric Research and the CDPHE to support the evaluation of MM5 near-surface temperature, water vapor, and wind speed fields. The specific NCAR data set used for this purpose was DS472.0 which is the hourly airways surface data. The primary data set available for comparing model performance aloft is the NOAA Forecast Systems Lab and National Climatic Data Center's Radiosonde Data of North America.

### 7.2.3 Evaluation Tools

The MM5 operational evaluation will include calculation and analysis of numerous statistical measures of model performance and the plotting of specific graphical displays to elucidate the basic performance of the model in simulating atmospheric variables. Tables 7-1 and 7-2 identify the specific statistical and graphical procedures that will be used to evaluate the MM5 model. These measures have been employed extensively in numerous other prognostic model evaluations (Seaman et al., 1997; Tesche et al., 2001a,b; Emery and Yarwood, 2001). The procedures are incorporated into the Model Performance Evaluation, Analysis, and Plotting Software (MAPS) system (McNally and Tesche, 1994) which will be used in this study.

## 7.3 Photochemical Model Evaluation Process

The CAMx performance evaluation will follow the procedures recommended in the EPA guidance documents (EPA, 1991; 1999). The evaluation will be carried out in two sequential phases, beginning with the simplest comparisons of modeled and observed ground-level ozone concentrations, progressing to potentially more illuminating analyses if necessary (e.g., examination of precursor and product species, comparisons of pollutant ratios and groupings). Below, we describe how this evaluation will be conducted using the MAPS software routines. Appendix A introduces several of the statistical and graphical procedures used in MAPS for meteorological and photochemical model evaluations. Details of the computational procedures and brief discussions of the EPA performance measures included in MAPS are presented in McNally and Tesche (1994a).

The procedures outlined in the draft 8-hour modeling guidance with respect to CAMx performance evaluation will be carried out in the Denver study. We will utilize all six means for assessing photochemical model performance as specified in the draft guidance are as follows:

> Use of computer generated graphics;
>
> Use of ozone metrics in statistical comparisons;
>
> Comparison of predicted and observed precursor emissions or species concentrations;
>
> Comparison of observed and predicted ratios of indicator species;
>
> Comparison of predicted source category contribution factors with estimates obtained using observational models; and
>
> Use of retrospective analyses in which air quality differences predicted by the model are compared with observed trends.

Obviously, a comprehensive measurement database for ozone and precursors from an extensive monitoring network is needed to support all six of these analyses. This is clearly not possible in the DNFFR region, particularly in regards to precursor measurements. Therefore, the approach to be followed for in this study will consist of a blend of those points above and the three basic model performance steps outlined below. To the extent possible, each of the performance procedures described by EPA's 8-hour guidance will be addressed, and at a minimum, an explanation of why certain components cannot be fulfilled will be provided.

Initial screening (Phase I) of the CAMx base case ozone predictions will be performed for the modeling episodes in an attempt to identify obviously flawed model simulations and to implement improvements to the model input files in a logical, defensible manner. If the screening phase suggests that no obvious flaws or compensating errors exist in the simulation(s), then one progresses to the operational evaluation. The screening evaluation will employ various ozone performance statistics and plots (listed in Table 7-3) developed with MAPS. Examples of the types of graphical displays to be considered for each base case include:

> Spatial mean ozone time series plots;
>
> Ozone time series plots;
>
> Ground-level ozone isopleths;
>
> Ozone concentration scatterplots;
>
> Bias and error stratified by concentration; and
>
> Bias and error stratified by time.

This screening is intended to identify obviously flawed simulations. Experience in photochemical modeling is the best basis upon which to identify obviously flawed simulation results. Efforts to improve photochemical model performance, where necessary and warranted (i.e., to reduce the discrepancies between model estimates and observations), should be based on sound scientific principles. A "curve-fitting" or "tuning" activity is to be avoided. The following principals should govern the model performance improvement process (to the fullest extent possible given the project schedule):

> Any significant changes to the model or its inputs must be documented;

> Any significant changes to the model or its inputs must be supported by scientific evidence, analysis of new data, or by re-analysis of the existing data where errors or misjudgments may have occurred;

> All significant changes to the model or its inputs should be reviewed by the project sponsors and/or other advisory group(s).

If the initial examination of the CAMx ozone results does not reveal obvious flaws, the formal operational evaluation (Phase II) follows. This activity consists of three steps. First, the graphical displays utilized in Phase I for ozone will be generated for NOx, the only available ozone precursor species in the Denver data base. Note that model performance for VOC species may not be tested since there are a limited quantity of relevant ambient VOC measurement data collected in the region.1 The graphical displays for this ozone precursor will be examined for obvious flaws. Should these be detected, the model diagnosis and performance improvement efforts may be needed to fully identify and correct (if possible) the noted problems. Second, the ozone and NOx predictions will be examined both at the ground and aloft. Where aloft data are lacking or in short supply, the modeled fields should nevertheless be examined to assess their reasonableness. Finally, a limited number of model sensitivity and/or uncertainty simulations may be performed to help elucidate model performance and response to changes in key inputs. Sensitivity analysis, often an important component of the evaluation process, may be performed to aid in understanding the CAMx's response to key input parameter uncertainties.

The extent to which sensitivity simulations with the CAMx will be needed can only be assessed after the initial model evaluations are performed. Note that with the advent of more sophisticated nested regional ozone models and input preprocessor models (MM5, EPS2x) a number of sensitivity runs historically carried out with the UAM-IV model are no longer feasible, needed, or appropriate (e.g., mixing height changes, zero-emissions runs). Other types of experiments have become potentially more useful (e.g., horizontal and vertical eddy diffusivity changes, vertical grid definition changes). Sensitivity experiments will be considered as part of the CAMx model performance evaluation analysis as appropriate. The potential need for and nature of these simulations would be discussed with the RAQC and the modeling subcommittee after the operational evaluation results have been reviewed.

[1] Some VOC speciation data may be available from EPA, the CDPHE, or other agencies. To the extent it is appropriate and available, that information will be examined.

**Table 7-1.** Statistical measures and graphical displays to be considered in the MM5 operational evaluation.

| Statistical Measure | Graphical Display |
|---|---|
| ***Surface Winds (m/s)*** | |
| Vector mean observed wind speed | Vector mean modeled and observed wind speeds as a function of time |
| Vector mean predicted wind speed | Scalar mean modeled and observed wind speeds as a function of time |
| Scalar mean observed wind speed | Modeled and observed mean wind directions as a function of time |
| Scalar mean predicted wind speed | Modeled and observed standard deviations in wind speed as a function of time |
| Mean observed wind direction | RMSE, $RMSE_s$, and $RMSE_u$ errors as a function of time |
| Mean predicted wind direction | Index of Agreement as a function of time |
| Standard deviation of observed wind speeds | Surface wind vector plots of modeled and observed winds every 3-hrs |
| Standard deviation of predicted wind speeds | Upper level wind vector plots every 3-hrs |
| Standard deviation of observed wind directions | |
| Standard deviation of predicted wind directions | |
| Total RMSE error in wind speeds | |
| Systematic RMSE error in wind speeds | |
| Unsystematic RMSE error in wind speeds | |
| Index of Agreement (I) in wind speeds | |
| $SKILL_E$ skill scores for surface wind speeds | |
| SKILLvar skill scores for surface wind speeds | |
| ***Surface Temperatures (Deg-C)*** | |
| Maximum region-wide observed surface temperature | Normalized bias in surface temperature estimates as a function of time |
| Maximum region-wide predicted surface temperature | Normalized error in surface temperature estimates as a function of time |
| Normalized bias in hourly surface temperature | Scatterplot of hourly observed and modeled surface temperatures |
| | Scatterplot of daily maximum observed |

| Statistical Measure | Graphical Display |
|---|---|
| Mean bias in hourly surface temperature | and modeled surface temperatures |
| Normalized gross error in hourly surface temperature | Standard deviation of modeled and observed surface temperatures as a function of time |
| Mean gross error in hourly surface temperature | Spatial mean of hourly modeled and observed surface temperatures as a function of time |
| Average accuracy of daily maximum temperature estimates over all stations | Isopleths of hourly ground level temperatures every 3-hr |
| Variance in hourly temperature estimates | Time series of modeled and observed hourly temperatures as selected stations |
| ***Surface Mixing Ratio (G/kg)*** | |
| Maximum region-wide observed mixing ratio | Normalized bias in surface mixing ratio estimates as a function of time |
| Maximum region-wide predicted mixing ratio | Normalized error in surface mixing ratio estimates as a function of time |
| Normalized bias in hourly mixing ratio | Scatterplot of hourly observed and modeled surface mixing ratios |
| Mean bias in hourly mixing ratio | Scatterplot of daily maximum observed and modeled surface mixing ratios |
| Normalized gross error in hourly mixing ratio | Standard deviation of modeled and observed surface mixing ratios as a function of time |
| Mean gross error in hourly mixing ratio | Spatial mean of hourly modeled and observed surface mixing ratios as a function of time |
| Average accuracy of daily maximum mixing ratio | Isopleths of hourly ground level mixing ratios every 3-hr |
| Variance in hourly mixing ratio estimates | Time series of modeled and observed hourly mixing ratios at selected stations |

**Table 7-2.** Statistical measures and graphical displays to be considered in the MM5 scientific evaluation. (measures and displays developed for each simulation day).

| Statistical Measure | Graphical Display |
|---|---|
| ***Aloft Winds (m/s)*** | |
| Vertically averaged mean observed and predicted wind speed aloft for each sounding | Vertical profiles of modeled and observed horizontal winds at each NWS sounding location and at each NOAA continuous upper-air profiler location in the 36, 12, and 4-km grid. |
| Vertically averaged mean observed and predicted wind direction aloft for each sounding | |
| ***Aloft Temperatures (Deg-C)*** | |
| Vertically averaged mean temperature observations aloft for each sounding | Vertical profiles of modeled and observed temperatures at each sounding location |
| Vertically averaged mean temperature predictions aloft for each sounding | |

**Table 7-3.** Statistical measures and graphical displays to be considered in the operational evaluation of CAMx.

| Statistical Measure | Graphical Display |
|---|---|
| Maximum observed concentration | Modeled and observed spatial mean concentrations as a function of time |
| Maximum modeled concentration | Measures of peak estimation accuracy ($A_{TS}$, $A_T$, $A_S$, $A_U$, A) |
| Maximum modeled concentration at a monitoring station | Normalized bias as a function of time |
| Ratio of maximum modeled to observed concentrations | Normalized gross error as a function of time |
| Accuracy of peak estimation (paired in time and space) | Normalized bias as a function of concentration level |
| Accuracy of peak estimation (unpaired in time and space) | Normalized gross error as a function of concentration level |
| Average accuracy over all stations | Scatterplot of hourly concentration pairs |
| Normalized bias in hourly concentrations | Scatterplot of daily maximum concentration pairs |
| Mean bias in hourly concentrations | Quartile plots of hourly species concentrations |
| Normalized gross error in hourly concentrations | Daily maximum ground-level concentration isopleths |
| Mean gross error in hourly concentrations | Time series of layer-integrated ozone and precursor species for each model level throughout the episode |
| Variance in hourly concentrations | |

Notes:
1. The chemical species to be considered include ozone, NO, $NO_2$, and $NO_x$ .
2. The chemical species ratios to be considered include $O_3/NO_y$, $O_3/NO_z$.
3. Graphical measures and statistical displays will be developed for each day of the episode.

# 8.0 8-HR OZONE ATTAINMENT DEMONSTRATION

## 8.1 Overview

This section summarizes the general approach to be followed in assessing whether the Denver Northern Front Range Region is likely to be in attainment of the 8-hr ozone standard or whether and to what extent additional VOC and/or NOx emissions reductions will be required to achieve attainment. Because EPA has not yet designated any region as non-attainment for 8-hr ozone, no formal requirement exists for an 8-hr attainment demonstration. Moreover, EPA is presently revising its draft 8-hr modeling guidance and the methodologies the agency has previously recommended in the 1999 draft guidance are being substantially revised. Consequently, in this protocol we present an “attainment demonstration” approach that is consistent with the current EPA draft guidance but allows for flexibility should refined guidance become available during the course of the Denver EAC study. The approach set forth below follows the main theme of the existing 8-hr guidance, e.g., use of station-specific relative reduction factors (RRFs) and Design Values (DVs), but does not prescribe the full set of screening analyses and weight of evidence (WOE) investigations that would attend a formal 8-hr ozone attainment demonstration. This is due, in part, because it is not apparent at this time that the region will be estimated to exceed the 8-hr standard in 2007.

The CAMx future-year (2007) baseline simulations for the Summer ’02 episode will reveal the extent to which further emissions reductions are needed in the region to provide for attainment of the 8-hr ozone NAAQS (EPA, 1999). Should ozone exceedances be modeled in the region in the future year baseline simulation, the severity, location, and spatial extent of the modeled exceedances will be studied in order to postulate candidate VOC and/or NOx emissions reductions strategies within and upwind of the nonattainment area. That is, should the future year modeling reveal a nonattainment problem, then a separate attainment demonstration analysis will be performed that will include the modeled attainment tests, specific screening analysis and supplemental corroborative analyses set forth in the EPA guidance.

## 8.2 Approach

EPA has developed draft procedures for using photochemical models to demonstrate attainment of the 8-hour ozone NAAQS. These procedures involve using the relative differences in the modeled 8-hour ozone estimates between a current year base case simulation (e.g., 1999) and a future year control scenario simulation (e.g., 2007) to scale the measured Design Value for comparison with the 84 ppb 8-hour ozone NAAQS. The EPA’s current guidance for using models to demonstrate attainment of the 8-hour ozone NAAQS will be adopted in this study. This includes the use of relative reduction factors, corroborative analyses (i.e., use of observational and other supportive information), weight-of-evidence determinations, and screening analyses necessary to address the specific characteristics of the three urban study areas.

## 8.3 Future Year Baseline Conditions

The future year baseline emissions inventory for 2007 will be obtained from the CDPHE and processed using the EPS2x modeling system to reflect the EPA-recommended source-category specific growth and control factors. The projected inventory will reflect the net effect of mandated controls and growth projections for each source category. Future-year boundary conditions on the perimeter of the 12 km Denver domain will be identical to those used in the base case performance evaluation runs. Since these conditions represent background Tropospheric ozone, VOC, and NOx concentrations advected across the 36 km coarse grid domain boundaries, there is expected to be little if any difference in these concentrations between the base years and the future forecast year. If necessary, CAMx model sensitivity experiments will be conducted to examine the reasonableness of this approach to boundary conditions. CAMx will be exercised for the future year 2007 using the appropriate initial conditions, boundary conditions, and emissions files. Model results will be interpreted statistically and graphically using the established software routines. Should modeled concentrations exceed the federal 8-hr standard within or downwind of the Denver-Northern Front Range region, it will be necessary to consider additional controls of VOC and/or NOx to bring the modeled results into attainment.

## 8.4 Development And Testing Of Candidate Emissions Control Strategies

At this time it is difficult to specify precisely the nature of any future year local Denver control scenario modeling inventories that might be required; indeed, we expect that the application of existing and mandated regional and local controls by the year 2007 will demonstrate that 8-hr attainment is, in all probability, demonstrated if not directly through photochemical modeling, then by a combination of modeling and weight of evidence analyses. Should future year control scenario modeling be required, the following general and specific principals would likely govern selection of appropriate scenarios to be developed.

## 8.5 Weight Of Evidence Analyses

The general purpose of the future year control scenario runs are to identify and evaluate possible controls based on available technologies and feasibility of implementation. If needed, we would begin by making focused emission-sensitivity simulations to refine the selection of control measures and their areas of applicability (e.g., local vs. regional). These sensitivity runs can be either traditional brute force (i.e., "across-the-board") runs, DDM emissions sensitivity runs, or both. Subsequently, we will develop inventories for use in more specific control-strategy simulations. These inventories would be developed to: (a) examine the effects of specific control measures, (b) examine the effects of packages of control measures, and (c) identify attainment strategy options such as alternative fuels, Inspection and Maintenance (I&M) programs at various levels, $NO_X$ "RACT" versus VOC "RACT", various transportation measures, proposed limits on agricultural activities, and so on. We would also consider control scenarios aimed at elucidating the sensitivity of regional versus subregional VOC and/or NOx controls. These simulations would examine the contribution from other states by reducing significantly their VOC and NOx anthropogenic emissions. General across-the-board simulations of VOC and/or NOx reductions (say 25% to 40%) from key subregions might be considered. We will also consider the impacts of VOC and NOx emissions reductions from different source categories (e.g., the effects of elevated vs. low-level $NO_X$ sources). We will also consider specific control programs but are not able to fully define them at the present time.

Up to twelve (12) year 2007 emissions sensitivity and general control scenario simulations will be considered, depending upon their aggregate level of complexity. Prior to executing such runs, however, we will submit list of priority-ranked options for RAQC's review and comment. It is assumed that approximately half the control scenarios will be across the board VOC and/or NOx emission reductions for a given subregion (or regionally) and a given source sector (e.g., on-road mobile sources, nonroad sources, point source, etc.), whereas the rest will be control measure specific strategies. The approved list of emissions control strategies will then constitute the set of future year control scenario inventories to be developed.

CAMx would be exercised for each of the future-year control strategies to estimate 2007 (or 2012) ozone levels under each control scenario. The EPA draft 8-hour ozone Design Value scaling procedures would be used to estimate future-year 8-hour ozone Design Values under the various control scenarios. The results of the future-year control strategies would entail: (a) tabular summary of the daily maximum 8-hour ozone concentrations in Denver, and the percent reduction from the 2007 Base Case scenario, (b) tabular summary of the projected 8-hour ozone Design Values in Denver, for the various control strategies and the percent reduction from the 2007 Base Case scenario, (c) spatial maps of daily maximum 8-hour ozone concentrations for each scenario, and (d) spatial maps of difference concentrations in 8-hour ozone concentrations between the 2007 control strategy and 2007 Base Case and other scenarios where appropriate.

## 8.6 Formal Ozone Attainment Demonstration

EPA's draft 8-hr attainment demonstration procedures involve the use of the relative differences in the modeled 8-hour ozone estimates between a current year base case simulation (e.g., 2002) and a future year control scenario simulation (e.g., 2007) to scale the measured design value for comparison with the 8-hour ozone NAAQS. We will employ this procedure using the EPA's Relative Reduction Factor (RRF) methodology with station-specific 8-hr ozone design values (DVs). We will also identify certain "weight of evidence" analyses (e.g., corroborative analyses, use of observational models and other supportive information, trends analyses, and other screening analyses) that may also be appropriate should a formal 8-hr ozone attainment demonstration be required for any of the three metropolitan areas.

EPA's guidance allows states to supplement photochemical grid modeling results with additional information designed to account for modeling uncertainties such as those affecting the model performance and response to controls. The process by which this is done is through a Weight of Evidence (WOE) determination. Under a WOE determination, EPA will consider a number of factors that may show a modeled control strategy is likely to achieve attainment even when attainment is not conclusively demonstrated by the modeling.

Innovative or unique approaches to demonstrating attainment through WOE may be needed, particularly for the Denver region, because the factors that govern the formation, accumulation, and ultimately the control of ozone may be somewhat different from those observed elsewhere. The density of stationary sources co-emitting $NO_x$ and reactive VOCs, plus the complex wind patterns and atmospheric vertical structures associated with Denver's mountain-basin meteorology, may result in complex spatial and temporal patterns of ozone may prove difficult to model accurately.

The draft 8-hr modeling guidance on WOE is notably flexible. While providing examples of analyses EPA will consider as components of a WOE determination, the guidance makes clear that additional factors may be considered on a case by case basis. The important thing to note about EPA's guidance on WOE is that its intent is to allow states to take into account uncertainties in the modeling process and provide evidence that a modeled control strategy is likely to produce attainment even when attainment is not conclusively demonstrated by the model. Additionally, current EPA's guidance contains no limit on how close the model must come to demonstrating attainment in order to conclude from other evidence that attainment is likely.

Possible components of a WOE determination to be explored in the Denver EAC study include:

- Assessment of model performance;
- Predicted changes in the ozone design value;
- Responsiveness of model predictions to additional controls;
- Results from other peer-reviewed photochemical grid models;
- Results from observational models;
- Analyses of air quality data;
- Additional controls not included in the modeling analysis
- Changes in the predicted frequency or pervasiveness of exceedances;
- Severity of the modeled episode;
- Air quality and emissions trend data, and
- Other analyses.

If the modeled attainment test to be applied in the Denver study narrowly misses the 8-hr NAAQS standard, additional focused analyses as part of a "weight of evidence" determination may be necessary. The specific analyses that might be considered, in addition to the diagnostic and process analyses previously mentioned, include:

- Calculation of the relative change in total grid-cell-hours across the DNFFR domain with maximum 8-hour ozone concentrations greater than or equal to 85 ppb;

> Calculation of the relative change in the number of grid cells across the DNFRR domain with 8-hour ozone concentrations greater than or equal to 85 ppb;

> Calculation of the relative change in the amount by which the 8-hour NAAQS is exceeded in the DNFRR domain by 8-hour simulated concentrations.

Significant reduction in these metrics would add support to the WOE analysis.

# 9.0 TECHNOLOGY TRANSFER

## 9.1 Reporting

Documents, technical memorandums, and data bases developed in this study will be submitted to the RAQC for review and subsequent distribution as appropriate. The various work products developed in preceding tasks will be synthesized and integrated to produce a draft Technical Support Document that describes the full range of technical and modeling activities performed during the project. This report will contain the essential methods and results of the conceptual model, episode selection, modeling protocol, base case model development and performance testing, future year and control strategy modeling, quality assurance, weight of evidence analyses, and calculation of 8-hr ozone attainment via EPA's relative reduction factor (RRF) methodology. We will work with the RAQC Project Officer to establish a suitable outline for the TSD. After receiving comments from the RAQC and other reviewers, we will prepare a final TSD document.

## 9.2 Data Archival

While the modeling results and supporting data bases will be immediately available to RAQC participants via the website or overnight transfer, the final project data delivery will be guided by the following principal: *All relevant data sets, model codes, scripts, and related software required by an independent peer-reviewer to corroborate the study findings (e.g., performance evaluations, control strategy runs) will be provided in an electronic format approved by RAQC*. Supplementing the data base delivery will be one or more CD's that provide easy-to-use graphics of the full suite of model evaluation and control strategy simulation results. The CD's will include color animations of the evolution of wind, thermodynamic, and pertinent gas-phase species fields over the study domain(s).

## 9.3 Transfer Of Modeling Data Files

Transfer of data within the ENVIRON/Alpine team and with the RAQC will be facilitated in part through the project website, and also through the routine transfer of large databases via overnight mail. Large database transfers will be accomplished using (a) the ftp protocol for smaller datasets, and (b) the use of IDE and firewire disk drives, allowing a transfer of 100s of Gb of data quickly and efficiently.

## 9.4 Training

The full suite of models and data bases developed in this study will be set up on CDPHE computers and a 3-day on-site training program will be offered in the use of the modeling system(s). The exact nature of the training courses will be developed through discussions between the study Team and CDPHE. The currently envisioned format consists of a blending of the issues/science involved with photochemical modeling studies and hands-on training using the models and databases used in this study. Topics could include the technical formulation, assumptions, input and output generation methodologies, and operation of the suite of current emissions models (e.g., EPS2x, EMS-2003, SMOKE, etc.), meteorological models (MM5), and photochemical/fine particulate models used in the study.

We envision that approximately one day (perhaps 1 ½ day) of the seminar would be conducted to provide a detailed overview of the fundamentals of photochemical, PM, and visibility modeling that would be appropriate for the emissions/air quality modeler as well as the air quality planners and others involved in the regulatory decision making process who need to understand the important aspects of photochemical modeling, without necessarily the details associated with operating the models on a computer. The first part of the training would also include model post-processing and analysis guidance to provide agency staff with the ability to interpret and critically analyze results of the model, and to effectively participate in new and on-going ozone, PM, and visibility modeling. This training would be supported by appropriate use and reference of the existing user's guides and technical formulation documents published by the developers of the various models. The second part of the training would be geared toward a two-day hands-on computer training on the major model components of the Denver air quality modeling system. Alpine Geophysics' Denver-based staff would install and test these components on the CDPHE computer systems prior to the training session.

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# APPENDIX A

# MODEL EVALUATION PROCEDURES

# A.0 OVERVIEW

Before the MM5/CAMx modeling system is applied to emission control strategy investigations for the Denver EAC study, it must be tested in accordance with EPA's model evaluation guidelines. This provides some assurance to decision-makers that the model is producing the right answer for the right reasons. EPA's recommended model evaluation process (EPA, 1991) includes the calculation and analysis of several routine statistical measures and the plotting of specific graphical displays to characterize the basic performance attributes of the model. Among the statistics examined are: different measures for characterizing the model's accuracy in estimating the maximum one-hour average concentration; mean normalized bias to indicate the degree to which calculated one-hour concentrations are over- or underestimated; the variance, describing the dispersion of the residual distribution about the mean; and the mean normalized gross error, which quantifies the average absolute signed deviation of the concentration residuals. Calculation of the EPA performance measures will be performed using the MAPS software, described briefly below.

The Model Performance Evaluation, Analysis, and Plotting Software (MAPS) system package was developed for urban- and regional-scale meteorological, emissions, and photochemical model evaluations. The MAPS system embodies a variety of the statistical and graphical model testing methods for photochemical and meteorological models recommended by various agencies including the California Air Resources Board (ARB) and the EPA (see, for example, ARB, 1992; EPA, 1991). MAPS also contains a variety of statistical and graphical tools for analyzing emissions model estimates. The performance measures calculated with MAPS are consistent with the definitions contained in Appendix C of the Guideline for Regulatory Application of the Urban Airshed Model.

MAPS consists of a set of special-purpose FORTRAN codes, the National Center for Supercomputer Applications (NCSA) Hierarchial Data Format (HDF) data management libraries (ported to SUN and IBM RS/6000 platforms) and National Center for Atmospheric Research (NCAR) Graphics, Version 3.01. The formulation of the general package of statistical measures and graphical procedures available within MAPS are presented in this appendix. Not all of these techniques will be used, however. In some of the definitions below, the variable $\Phi$ represents a model-estimated or derived quantity, e.g., wind speed, wind direction, PBL height, ambient temperature. The subscripts e and o correspond to model-estimated and observed quantities, respectively. The subscript i refers to the ith hour of the day.

## A.1 MEAN AND GLOBAL STATISTICS

Several statistical measures are calculated to provide an overall summary of photochemical and meteorological model estimates and observations and to support calculation of other statistical measures.

**Mean Estimation ($M_e$).** The mean model estimate is given by:

$$M_e = \frac{1}{N}\sum_{i=1}^{N} \Phi_{ei}$$

where N is the product of the number of simulation hours and the number of ground-level monitoring locations providing hourly-averaged observational data. $\Phi_{ei}$ represents the model-estimate at hour i.

**Mean Observation ($M_o$).** The mean observation is given by:

$$M_o = \frac{1}{N}\sum_{i=1}^{N} \Phi_{oi}$$

Here, $\Phi_{oi}$ represents the observations at hour i.

**Average Wind Direction.** Because wind direction has a crossover point between 0 degrees and 360 degrees, standard linear statistical methods cannot be used to calculate the mean or standard deviation. Evaluations by the EPA (Turner, 1986) suggest that the method proposed by Yamartino (1984) performs well in estimating the wind direction standard deviation. Specifically, this quantity is calculated by:

$$\sigma_\alpha = \arcsin(\beta)\ [1 + 0.1547\ \beta^3]$$

where:

$$\beta = \left[\ 1.0 - \ [(\overline{\sin\ \alpha})^2 + (\overline{\cos\ \alpha})^2\ ]\ \right]^{1/2}$$

Here, alpha is the measured hourly or instantaneous wind direction value.

**Standard Deviation of Estimation (Sde).** The standard deviation of the model estimates is given
by:

$$SD_e = \left[\ \frac{1}{N}\sum_{i=1}^{N} |\Phi_{ei} - M_e|^2 \right]^{1/2}$$

**Standard Deviation of Observations (SDo).** The standard deviation of the observations is given by:

$$SD_o = \left[\ \frac{1}{N}\sum_{i=1}^{N} |\Phi_{oi} - M_o|^2 \right]^{1/2}$$

**Least Square Slope and Intercept Regression Statistics.** A linear least-squares regression is performed to calculate the intercept (a) and slope (b) parameters in the following equation:

$$\hat{\Phi}_{ei} = a + b \;\; \Phi_{oi}$$

This regression is performed for each set of hourly (or instantaneous) data to facilitate calculation of several error and skill statistics.

**Maximum Ratio ($R_{max}$).** The maximum ratio is defined as the quotient of the maximum one-hour averaged model estimated concentration and the maximum hourly-averaged measurement, i.e.,

$$R_{\max} = \frac{c_e(x,t)}{c_o(\hat{x},\hat{t})}$$

where $c_e$ is the estimated one-hour averaged pollutant concentration, $c_o$ is the observed hourly averaged concentration, $\hat{x}$ refers to the peak monitoring station location, $\hat{t}$ is the time of the peak observation. The caret, ˆ, denotes the time or location of the maximum observed concentration. There is no requirement that the maximum estimated and observed concentrations be paired in either time or space but for this measure we require that the maximum modeled concentration be taken from a monitoring station.

## A.2 DIFFERENCE STATISTICS

**Residual ($d_i$).** For quantities that are continuous in space and time (i.e., wind speed, temperature, pressure, pbl height, species concentrations) difference (or residual) statistics are very useful. Difference statistics are based on the definition of a residual quantity. A concentration residual, for example, is defined as:

where $d_i$ is th $d_i = c_e(x_i,t) - c_o(x_i,t)$

e i-th residual based on the difference between model-estimated ($c_e$) and observed ($c_o$) concentration at location x and time i.

**Standard Deviation of Residual Distribution (SDr).** The standard deviation of the residual distribution is given by:

$$SD_r = \left( \frac{1}{N-1} \sum_{i=1}^{N} (d_i - MBE)^2 \right)^{0.5}$$

where the concentration residual is defined as:

$$d_i = c_e(x_i,t) - c_o(x_i,t)$$

and MBE is the first moment, i.e., the mean bias error, defined shortly. This statistic describes the "dispersion" or spread of the residual distribution about the estimate of the mean. The standard deviation is calculated using all estimation-observation pairs above the cutoff level. The second moment of the residual distribution is the variance, the square of the standard deviation. Since the standard deviation has units of concentration, it is used here as the metric for dispersion. The standard deviation and variance measure the average "spread" of the residuals, independent of any systematic bias in the estimates. No direct information is provided concerning subregional errors or about large discrepancies occurring within portions of the diurnal cycle although in principle these, too, could be estimated.

**Accuracy of Peak Model Estimates (A).** Five related methods are used to evaluate the accuracy of the model's estimate of the maximum value of a spatially-distributed variable. This may be, for example, temperature, wind speed, pressure, or concentration. In the definitions below we use the peak one-hour average concentrations for discussion purposes; however, these measures may be applied to several of the meteorological variables as well.

Several accuracy measures are used because there are different, informative, and plausible ways of comparing the peak measurement on a given day with model estimates. These five accuracy measures provide complimentary tests of the model's performance. When applied to ozone simulations, they are particularly useful from a regulatory perspective since they deal with peak ozone (or precursor) concentration levels.

Paired Peak Estimation Accuracy. The paired peak estimation accuracy, $A_{ts}$, is given by:

$$A_{ts} = \frac{c_e(\hat{x},\hat{t}) - c_o(\hat{x},\hat{t})}{c_o(\hat{x},\hat{t})} 100\,\%$$

$A_{ts}$ quantifies the discrepancy between the magnitude of the peak one-hour average concentration measurement at a monitoring station, $c_o(\hat{x},\hat{t})$, and the estimated concentration at the same location, $\hat{x}$, and at the same time, $\hat{t}$. Model estimates and observations are thus "paired in time and space." The paired peak estimation accuracy is a stringent model evaluation measure. It quantifies the model's ability to reproduce, at the same time and location, the highest observed concentration during each day of the episode. The model-estimated concentration used in all comparisons with observations is derived from bi-linear interpolation of the four ground level grid cells nearest the monitoring station.

$A_{ts}$ is very sensitive to spatial and temporal misalignments between the estimated and observed concentration fields. These space and time offsets may arise from spatial displacements in the transport fields resulting from biases in wind speed and direction, problems with the "timing" of photochemical oxidation and removal processes, or subgrid-scale phenomena (e.g., ozone titration by local $NO_x$ emission sources) that are not intended to be resolvable by grid-based photochemical models.

Temporally-Paired Peak Estimation Accuracy. The temporally-paired peak estimation accuracy, $A_t$, is given by:

$$A_t = \frac{c_e(x,\hat{t}) - c_o(\hat{x},\hat{t})}{c_o(\hat{x},\hat{t})} \; x\,100\,\%$$

$A_t$ quantifies the discrepancy between the highest concentration measurement at a monitoring station and the highest model estimate at the same station or any other grid cell within a distance of, say, 4 -5 grid cells. This measure examines the model's ability to reproduce the highest observed concentration in the same subregion at the correct hour.

Spatially-Paired Peak Estimation Accuracy. The spatially-paired peak estimation accuracy, $A_s$, is given by:

$$A_s = \frac{c_e(\hat{x},t) - c_o(\hat{x},\hat{t})}{c_o(\hat{x},\hat{t})} \; x\,100\,\%$$

$A_s$ quantifies the discrepancy between the magnitude of the peak one-hour average concentration measurement at a monitoring station and the highest estimated concentration at the same monitor, within 3 hours (before or after) the peak hour.

Unpaired Peak Estimation Accuracy. The unpaired peak estimation accuracy, $A_u$,
is given by:

$$A_u = \frac{c_e(x,t) - c_o(\hat{x},\hat{t})}{c_o(\hat{x},\hat{t})} \; x\,100\,\%$$

$A_u$ quantifies the difference between the magnitude of the peak one-hour average measured concentration and the highest estimated value in the modeling domain, whether this occur at a monitoring station or not. The unpaired peak estimation accuracy tests the model's ability to reproduce the highest observed concentration anywhere in the region. This is the least stringent of the above four peak estimation measures introduced thus far. It is a weak comparison relative to the previous ones but is useful in coarse screening for model failures. This measure quickly identifies situations where the model produces maximum ozone concentrations in the air basin that significantly exceed the highest observed values within the network.

Average Station Peak Estimation Accuracy. The average station peak estimation accuracy, $\underline{A}$, is given by:

$$\overline{A} = \frac{1}{N} \sum_{i=1}^{N} |A_{si}|$$

where:

$$A_{si} = \frac{c_e(\hat{x}_i, t) - c_o(\hat{x},\hat{t})}{c_o(\hat{x},\hat{t})} \; x\,100\,\%$$

Here, $x_i$ is the ith monitoring station location. $\underline{A}$ is calculated by first determining the spatially-paired peak estimation accuracy, Asi, at each monitoring station. Thus, the average station peak estimation accuracy is simply the mean of the absolute value of the $A_{si}$ scores, where the temporal offset between estimated and observed maxima at any monitoring station does not exceed three hours.

**Mean Bias Error (MBE).** The mean bias error is given by:

$$MBE = \frac{1}{N}\sum_{i=1}^{N}(c_e(x_i, t) - c_o(x_i, t))$$

where N equals the number of hourly estimate-observation pairs drawn from all valid monitoring station data on the simulation day of interest.

**Mean Normalized Bias Error (MNBE).** The mean normalized bias error, often just called the bias, is given by:

$$MNBE = \frac{1}{N}\sum_{i=1}^{N}\frac{(c_e(x_i,t) - c_o(x_i,t))}{c_o(x_i,t)} \text{ x } 100\ \%$$

Mathematically, the bias is derived from the average signed deviation of the concentration residuals and is calculated using all pairs of estimates and observations above the cutoff level.

Cutoff levels of 40-60 ppb for ozone and 20 ppb for $NO_2$ are often used in modeling studies to reduce the influence that low measured or modeled concentrations (often occurring at night or on the upwind boundaries) have on the normalized bias statistics. In regions of exceptionally high ozone, e.g., the South Coast Air Basin, cutoff levels as high as 100 ppb are commonly used. For this study, an ozone cutoff level of 60 ppb will be used, consistent with EPA (1991) guidance.

**Mean Absolute Gross Error (MAGE).** The mean gross error is calculated in two ways, similar to the bias. The mean absolute gross error is given by:

$$MAGE = \frac{1}{N}\sum_{i=1}^{N}|c_e(x_i, t) - c_o(x_i, t)|$$

**Mean Absolute Normalized Gross Error (MANGE).** The mean absolute normalized gross error is:

$$MANGE = \frac{1}{N}\sum_{i=1}^{N}\frac{|c_e(x_i, t) - c_o(x_i, t)|}{c_o(x_i, t)} \text{ x } 100\ \%$$

The gross error quantifies the mean absolute deviation of the concentration residuals. It indicates the average unsigned discrepancy between hourly estimates and observations and is calculated for all pairs above the cutoff level of 60 ppb. Gross error is a robust measure of overall model performance and provides a useful basis for comparison among model simulations across different air basins or ozone episodes. Unless calculated for specific locations or time intervals, gross error estimates provide no direct information about sub-regional errors or about large discrepancies occurring within portions of the diurnal cycle.

**Root Mean Square Error (RMSE).** The root mean square error is given by:

$$RMSE = \left[ \frac{1}{N} \sum_{i=1}^{N} \left| \Phi_{ei} - \Phi_{oi} \right|^{2} \right]^{1/2}$$

The RMSE, as with the gross error, is a good overall measure of model performance. However, since large errors are weighted heavily, large errors in a small subregion may produce large a RMSE even though the errors may be small elsewhere.

**Systematic Root Mean Square Error ($RMSE_S$).** A measure of the model's linear (or systematic) bias may be estimated from the systematic root mean square error given by:

$$RMSE_s = \left[ \frac{1}{N} \sum_{i=1}^{N} \left| \hat{\Phi}_{ei} - \Phi_{oi} \right|^{2} \right]^{1/2}$$

**Unsystematic Root Mean Square Error ($RMSE_u$).** A measure of the model's unsystematic bias is given by the unsystematic root mean square error, that is:

$$RMSE_u = \left[ \frac{1}{N} \sum_{i=1}^{N} \left| \Phi_{ei} - \hat{\Phi}_{ei} \right|^{2} \right]^{1/2}$$

The unsystematic difference is a measure of how much of the discrepancy between estimates and observations is due to random processes or influences outside the legitimate range of the model.

A "good" model will provide low values of the root mean square error, RMSE, explaining most of the variation in the observations. The systematic error, $RMSE_S$ should approach zero and the unsystematic error $RMSE_u$ should approach RMSE since:

$$RMSE^2 = (RMSE_s)^2 + (RMSE_u)^2$$

It is important that RMSE, $RMSE_s$, and $RMSE_u$ are all analyzed. For example, if only RMSE is estimated (and it appears acceptable) it could consist largely of the systematic component. This bias might be removed, thereby reducing the bias transferred to the photochemical calculation. On the other hand, if the RMSE consists largely of the unsystematic component ($RMSE_u$), this indicates further error reduction may require model refinement and/or data acquisition. It also provides error bars that may used with the inputs in subsequent sensitivity analyses.

## A.3 SKILL MEASURES

**Index of Agreement (I).** Following Willmont (1981), the index of agreement is given by:

$$I = 1 - \left[ \frac{N \ (RMSE)^{\ 2}}{\sum_{i=1}^{N} \left( |\Phi_{ei} - M_o| + |\Phi_{oi} - M_o| \right)^2} \right]$$

This metric condenses all the differences between model estimates and observations into one statistical quantity. It is the ratio of the cumulative difference between the model estimates and the corresponding observations to the sum of two differences: between the estimates and observed mean and the observations and the observed mean. Viewed from another perspective, the index of agreement is a measure of how well the model estimates departure from the observed mean matches, case by case, the observations' departure from the observed mean. Thus, the correspondence between estimated and observed values across the domain at a given time may be quantified in a single metric and displayed as a time series. The index of agreement has a theoretical range of 0 to 1, the latter score suggesting perfect agreement.

**RMS Skill Error ($Skill_e$).** The root mean square error skill ratio is defined as:

$$Skill_E = \frac{RMSE_u}{SD_o}$$

**Variance Skill Ratio ($Skill_{var}$).** The variance ratio skill is given by:

$$Skill_{Var} = \frac{SD_e}{SD_o}$$

## A.4 GRAPHICAL TOOLS

Many features of CAMx and meteorological model simulations are best analyzed through graphical means. In addition to revealing important qualitative relationships, graphical displays also supply quantitative information. The main graphical displays that may be used to analyze CAMx performance results are as follows:

> The relationships among the five accuracy measures;

> The temporal correlation between estimates and observations;
> The spatial distribution of estimated concentration fields;

> The correlation among hourly pairs of estimates, observations and residuals;

> The variation in bias and error estimates as functions of time and space; and

> The degree of mismatch between volume-averaged model estimates and point measurements.

> The distributional relationships between rank-ordered observations and rank-ordered model estimates.

Brief discussions of these plotting method are as follows.

**Accuracy Plots**. Two accuracy plots are used. One depicts relationships between the peak five accuracy measures while the other plot summarizes the peak estimation accuracy at all monitoring stations, revealing the presence of subregional estimation bias if it occurs. The first plot is a histogram that displays the calculated values of $A_{ts}$, $A_t$, $A_s$, $A_u$, and $\underline{A}$. The second plot is also a histogram showing the peak observed and estimated concentrations (unpaired in time) at each monitoring station above the cutoff concentration of 60 ppb. Also contained on the plot is a shaded region corresponding to the normalized gross error.

**Time Series Plots**. Probably the most useful graphical procedure for depicting air quality model results is the time series plot. Developed for each monitoring station for which observed concentrations are available, this plot presents the hourly estimates and observations throughout the simulation period. The time series plot consists of the hourly averaged observations (boxes) and the hourly averaged estimates, the latter being fitted by a smooth continuous line. The model estimates are derived from bi-linear interpolation of the nearest four grid cells to the monitor. At each hour, the absolute value of the concentration residual will be calculated and plotted as a dashed line on the same plot.

With the time series plot one may determine the model's ability to reproduce the peak estimation, the presence or absence of significant bias and errors within the diurnal cycle, and whether the "timing" of the estimated concentration maximum agrees with the observation. By including the residual plot on the same graph, estimation biases are more apparent.

**Spatial Time Series Plots**. Conventional time series plots do not reveal situations where the model estimates concentrations comparable in magnitude to the observations a short distance away from the monitoring station. A second time series display, called a "spatial time series plot", are used for this purpose. These plots provide information about the degree to which model discrepancies result from the procedure for selecting the estimated values. There is no a priori reason to select the four-cell bi-linear average estimate over the estimate in the specific grid cell containing the monitor (i.e., the "cell value"), or perhaps the grid cell estimate within any of the four adjacent cells that is closest in magnitude to the observed value (i.e. the "best" estimate). Spatial time series plots are constructed for each monitoring station by plotting the hourly observations together with an envelope defined by the highest and lowest grid cell estimate within one cell of the monitoring station. MAPS can easily examine multiple grid cell distances as well.

The spatial time series plots provide diagnostic information about the "steepness" of the concentration gradients in the simulated fields. A small envelope indicates relatively flat concentration gradients. Conversely, steep gradients may produce a fairly large envelope. Ideally, the measurement points will fall within the envelope. Spatial time series plots are one method of revealing the correspondence or "commensurability" between volume-averaged model estimates and point measurements.

**Ground Level Isopleths**. Ground-level ozone isopleths are developed for each hour of the episode to display the spatial distribution of estimated concentration fields. The isopleth plots are developed by computer-contouring the hourly, gridded ozone estimates. The information content of these plots are enhanced by including the following:

> A base map identifying significant geophysical and political boundaries;

> Locations of air monitoring stations;

> The observed concentrations at each monitoring station by a bold numeral;

> The location of the peak estimate (signified by an asterisk); and

> The magnitude of the peak grid cell estimate.

Ground-level isopleths are also constructed based on the daily maximum concentration estimate in each grid cell. These "maximum" ozone isopleths supply direct information about the magnitude and location of pollutant concentrations and help to identify situations where sub-regional biases may be attributed to spatial misalignment of the estimated and observed concentration fields.

**Scatterplots of Estimates and Observations**. Scatterplots are a useful means of visually assessing the extent of bias and error in hourly ozone estimate-observation pairs. Hourly scatterplots are developed by plotting all hourly-averaged estimate-observation pairs for which the observed concentration exceeds the cutoff value. Similarly, daily maximum scatterplots are developed from the pairs of maximum hourly estimated and observed values at each monitoring station. The estimated maximum is the highest value simulated within three hours of the observed maximum. In these plots, the solid diagonal line with 1:1 slope will be used to identify the perfect correlation line and the dashed lines enclose the region wherein estimates and observations agree to within a factor of two. The lines of agreement can be made more stringent if desired.

The scatterplot is used to give a quick visual indication of the extent of over-or underestimation in the hourly estimates and whether there appear to be strong nonlinearities in model estimates and observations over the concentration range studied. Bias is indicated by the preponderance of data points falling above or below the perfect correlation line. The dispersion (spread) of points provides a visual indication of the general error pattern in the simulation. Scatterplots help identify outlier estimate-observation pairs, i.e., a seemingly discrepant estimate-observation pair that may result from erroneous data, a fundamental flaw in the model, or some other cause that requires investigation. These plots provide little diagnostic information about sub-regional performance problems, temporal or spatial misalignments, or other inadequacies in the simulation. In addition, scatterplots mask the temporal correlation between various estimate-observation pairs.

**Scatterplot of Residuals and Observations.** Residual scatterplots are developed to describe the distribution of hourly average model discrepancies (positive and negative) as a function of concentration level. This graphical display is constructed from the data elements that make up the bias and error calculations. Hourly concentration residuals for all monitoring stations are plotted as a function of observed concentration for all pairs above the cutoff value. A daily maximum residual plot is also constructed based on data pairs involving the maximum observed concentration at a monitor station and the maximum estimated value at the same station within three hours of the peak.

Residual scatterplots are used to characterize estimation discrepancy throughout the observed concentration range. The plot does not reveal the existence or causes of sub-regional or timing performance problems. Absence of bias is suggested by no systematic tendency for the data points to fall above or below the ordinate; however, as noted previously, important subregional biases may still exist in the presence of a zero overall bias estimate.

**Bias Stratified by Concentration.** Bias-concentration plots are derived from the residual distribution to depict the degree of systematic bias in hourly-averaged model estimates (paired in time and space) as a function of observed concentration level. This plot (and the companion error-concentration plot) aids in model diagnosis. The observed concentration range is divided into several equal-sized concentration bins and the normalized bias within each bin is calculated and plotted as a function of concentration level. A smooth line is then fitted through the bin-averaged values. The bias-concentration plot is used to reveal the existence of under- or over-estimation throughout the concentration range.

**Gross Error Stratified by Concentration.** Gross error-concentration plots is derived from the residual distribution to depict the error in model estimation (paired in time and space) as a function of observed concentration level. The observed concentration range is divided into several equal-sized concentration bins. Then, the average value of the normalized gross error within each bin is calculated and the bin averages are plotted as a function of the observed concentration level. MAPS will display the mean normalized gross error on the plot for easy reference.

The gross error-concentration plot is used to reveal the variation in model error at various intervals throughout the concentration range. The plot must be interpreted carefully, however, remembering that the concentration residual is normalized by the observed value.

**Bias Stratified by Time.** Bias-time plots are developed to help identify specific time periods within the photochemical simulation when systematic patterns of under- or overestimation occur. The bias-time plot is constructed in a manner similar to the bias-concentration plot, except that the simulation period is discretized into a number of time intervals, usually 1-2 hours in duration. Systematic bias in model estimates during specific periods within the diurnal cycle may have several causes: biases in vertical mixing or wind transport; "timing" problems with the chemistry; non-representative temporal distributions assumed in the emissions inventory, and so on. While the bias-time plots may not clearly pinpoint the causes of bias, they may be helpful in defining the time intervals when the bias is most apparent. This helps focus subsequent diagnostic investigations.

**Gross Error Stratified by Time.** Gross error-time plots are developed to help identify specific time periods when gross errors in the model estimates may be a problem. This plot is constructed in a similar manner as the error-concentration plot, except that the simulation period is discretized into a number of time intervals, usually 1-2 hours in duration. When interpreting the gross error-time and bias-time plots, one must remember that the concentration levels of all pollutants vary throughout the diurnal cycle.

**Quantile-Quantile Plots.** Quantile-quantile plots are cumulative frequency distributions that provide a graphical characterization of the distribution of observed and modeled values over their entire ranges. Quantitative information that can be obtained from these distributions include estimates of the mean, median, and standard deviation. The plots also provide a visual characterization of how the estimates and observations are spread out with respect to the central value. They also readily display unpaired bias.