Draft Final Report

MODELING PROTOCOL FOR THE DENVER 8-HOUR OZONE ATTAINMENT DEMONSTRATION MODELING

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November 28, 2007

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1.0 INTRODUCTION

1.1 Overview

This report constitutes the Air Quality Modeling Protocol for the Denver Metropolitan Area (DMA) and adjacent regions 8-hour ozone modeling analysis in support of the development of an 8-hour ozone State Implementation Plan (SIP) and attainment demonstration. This protocol describes the overall modeling activities to be performed in order to demonstrate attainment of the 8-hour ozone standard in the DMA and adjacent areas in Colorado. The DMA 8-hour ozone modeling is being carried out by a contracting team of ENVIRON International Corporation and Alpine Geophysics, LLC (Alpine) (the modeling team) under contract to the Denver Regional Air Quality Council (RAQC) which is the lead agency for this project. Providing assistance to the RAQC are the Colorado Department of Public Health and Environment (CDPHE), Denver Regional Council of Governments (DRCOG), Colorado Department of Transportation (CDOT) and the Northern Front Range Metropolitan Planning Organization (NFRMPO).

A comprehensive modeling protocol for an 8-hour ozone SIP attainment demonstration study consists of many elements. Its main function is to serve as a means for planning and communicating how a modeled attainment demonstration will be performed before it occurs. The protocol guides the technical details of a modeling study and provides a formal framework within which the scientific assumptions, operational details, commitments and expectations of the various participants can be set forth explicitly and means for resolution of potential differences of technical and policy opinion can be worked out openly and within prescribed time and budget constraints.

As noted in the U.S. Environmental Protection Agency's (EPA) 8-hour ozone modeling guidance, the modeling protocol serves several important functions (EPA, 2007):

- Identify the assistance available to the RAQC and APCD (the lead agencies) to undertake and evaluate the analysis needed to support a defensible attainment demonstration;
- Identify how communication will occur among State, Local and Federal agencies and stakeholders to develop a consensus on various issues;
- Describe the review process applied to key steps in the demonstration; and
- Describe how changes in methods and procedures or in the protocol itself will be agreed upon and communicated with stakeholders and the appropriate U.S. EPA regional Office.

1.2 Study Background

Ozone air quality in the DMA has been near the 8-hour ozone National Ambient Air Quality Standard (NAAQS) of 0.08 ppm (exceedance defined by values of 85 ppb and higher). In December 2002, the RAQC and APCD and others entered into an 8-hour ozone Early Action Compact (EAC) with the U.S. Environmental Protection Agency (EPA). EPA's EAC allows an area to submit an enforceable 8-hour ozone SIP by March 2004 that demonstrates attainment of the 8-hour ozone standard by 2007. In return EPA will defer the classification of an area as nonattainment until 2007. The RAQC and APCD contracted with ENVIRON and Alpine to do the photochemical modeling necessary for the Denver 8-hour ozone EAC. At the outset of the EAC modeling, Denver attained the 8-hour ozone NAAQS. However, the monitored ozone concentrations during the summer of 2003 resulted in violations of the 8-hour ozone standard. Because of the EAC, EPA designated the DMA 8-hour ozone classification as "nonattainment deferred" with final designation to be determined after the 2007 ozone season. More details on the Denver 8-hour EAC SIP are available at:

- http://www.raqc.org/ozone/EAC/ozone-eac.htm

Ozone attainment is based on 8-hour ozone Design Values (DVs) that are defined as the three-year average of the fourth highest 8-hour ozone concentration during a year at a monitor. Based on measured ozone concentrations during 2005-2007, the maximum 8-hour ozone DV in the DMA was 85 ppb at the Rocky Flats North (RFNO) monitoring site, which exceeds the 8-hour ozone NAAQS. Consequently, EPA is expected to designate the DMA as nonattainment for 8-hour ozone and the RAQC/APCD will need to develop an 8-hour ozone SIP that demonstrates the DMA will achieve attainment of the 8-hour ozone NAAQS by 2010.

On June 20, 2007, EPA proposed new primary and secondary ozone NAAQSs that would likely be more stringent than the current 8-hour ozone NAAQS of 85 ppb. EPA requested comments on a proposed new 8-hour ozone NAAQS with thresholds in the 0.070 ppm to 0.075 ppm range (70-75 ppb) or whether they consider values as low as 0.060 ppm (60 ppb) or keep the threshold at the current 0.08 ppm (85 ppb) level. Of the ~14 ozone monitors in the greater DMA, half have 2005-2007 8-hour ozone DVs that are 75 ppb or higher and all of them, except the downtown Denver CAMP monitor, have 8-hour ozone DVs of 70 ppb or higher.

1.3 Lead Agency and Principal Participants

The Denver RAQC and CDPHE/APCD are the lead agencies in the development of the Denver 8-hour ozone SIP. Additional participants include the Denver Regional Council of Governments (DRCOG), the Colorado Department of Transportation (CDOT), Northern Front Range Metropolitan Planning Organization (NFRMPO), and the Colorado Air Quality Control Commission (AQCC). EPA Region 8 in Denver is the local regional EPA office that will take the lead in the approval process for the Denver 8-hour ozone SIP. The RAQC has contracted with ENVIRON International Corporation with their subcontractor Alpine Geophysics, LLC (the modeling team) to assist them and the APCD in the 8-hour ozone attainment modeling demonstration.

1.4 Related Regional Modeling Studies

There are several additional ozone modeling studies that are nearby and related to the Denver 8-hour ozone modeling analysis whose results may be useful to the Denver 8-hour ozone modeling.

1.4.1 EPA Regional Regulatory Air Quality Programs

There are several EPA regional regulatory air control initiatives that have either a direct or indirect relevance to the Denver 8-hour ozone attainment demonstration SIP. These issues include, but are not limited to, the following:

Clean Air Interstate Rule (CAIR): Although the State of Colorado is not part of the CAIR control region for ozone and/or $PM_{2.5}$ that focuses on the eastern U.S. (e.g., Texas, Missouri, Illinois, Wisconsin and Minnesota eastwards), when flow is from the east the CAIR controls will likely reduce ozone transport into the DMA somewhat.

Clean Air Mercury Rule (CAMR): Colorado Electrical Generating Units (EGU) are subject to the requirements of the Clean Air Mercury Rule (CAMR).

Clean Air Visibility Rule (CAVR): The Clean Air Visibility Rule (CAVR) requires specific sources that are shown to reasonably contribute to visibility impairment at a Class I area to install Best Available Retrofit Technology (BART). The BART requirements apply to sources built between 1962 and 1977 that have the potential to emit 250 tons per year (TPY) of a visibility impairing pollutants (SO2, NOx, PM and/or VOC) and are one of 26 specific source categories. EPA has published guidelines for the BART component of the CAVR (EPA, 2005c). The APCD has published BART rules that would reduce NOx and SO2 emissions from several large sources that may contribute to ozone concentrations in the DMA so would benefit the Denver 8-hour ozone problem. Details on the Colorado BART rule making can be found at:

- http://www.cdphe.state.co.us/ap/RegionalHazeBART.html

1.4.2 Denver EAC SIP Modeling

The Denver EAC SIP modeling discussed previously performed 36/12/4/1.33 km photochemical modeling of the DMA using the MM5 meteorological, EPS3 emissions and CAMx photochemical grid models and a summer 2002 period (see: http://www.raqc.org/ozone/EAC/ozone-eac.htm). Although the EAC SIP modeling used grid spacing as small as 1.33 km and noted improved meteorological performance at the finer grid spacing, there were little benefits in the photochemical modeling using the 1.33 km versus 4 km grid spacing. In fact ozone model performance degraded somewhat using the 1.33 km grid and the computational requirements increased substantially. Based on these findings the current Denver 8-hour ozone modeling is not going down to use a 1.33 km grid and will use a 4 km grid for the DMA.

1.4.3 WRAP Regional Modeling Center Modeling

Five Regional Planning Organizations (RPOs) are performing regional haze modeling using photochemical ozone and PM models to support the development of regional haze SIPs due December 2007. The Western Regional Air Partnership (WRAP) is the RPO for the western states and the modeling is being conducted by the Regional Modeling Center (RMC) that consists of the University of California at Riverside (UCR), ENVIRON International Corporation and the University of North Carolina (UNC). The RMC has conducted modeling for the 2002 annual period and continental U.S. using a 36 km grid and the MM5 meteorological

(Kemball-Cook et al., 2005), SMOKE emissions and CMAQ and CAMx photochemical models. CMAQ was run for a 2002 base case 2018 future base-year and 2018-control scenarios to predict visibility projections in the Federal Class I areas. The WRAP RMC has a website where modeling results can be obtained and some of the modeling results have been implemented in the WRAP Technical Support System (TSS) website where users can analyze data and modeling results. These websites are at:

- http://pah.cert.ucr.edu/aqm/308/index.shtml
- http://vista.cira.colostate.edu/tss/

1.4.4 Four Corners Air Quality Task Force

The Four Corners Air Quality Task Force (FCAQTF) is conducting emissions and photochemical grid modeling of the four corners area to provide information regarding ozone, visibility and deposition impacts in the region. The states of Colorado and New Mexico are active participants in the FCAQTF. The SMOKE emissions and CAMx air quality models are being applied on a 36/12/4 km grid with the 4 km grid focused on northwest New Mexico, southwest Colorado and small portions of southeast Utah and northeast Arizona. This region not only includes the San Juan basin oil and gas development area but several large coal-fired power plants as well (Four Corners and San Juan). The FCAQTF is performing 2005 base case modeling as well as 2018 future-year modeling and 2018 sensitivity modeling of several mitigation scenarios. More details on the FCAQTF modeling can be found at:

- http://www.nmenv.state.nm.us/aqb/4C/PublicReview.html

1.4.5 Environmental Impact Statements (EISs) and Related Modeling

Photochemical grid models are also being applied in the general vicinity of the DMA as part of the development of Environmental Impact Statements (EISs) for oil and gas development projects. The Bureau of Land Management (BLM) has recently completed draft EISs for the Moxa Arch, Hiawatha and Pinedale Anticline gas infill projects in southwestern Wyoming that used the CAMx photochemical grid model with a 36/12/4 km grid to model the 2002 annual period and assess the potential ozone impacts due to the cumulative oil and gas development projects in southwestern Wyoming. A new BLM oil and gas production GIS has been initiated (Continental Divide – Creston) that will evaluate both the CMAQ and CAMx models and then run for 2002, 2005, and 2006. Additional BLM EISs will likely continue to use photochemical grid models for such ozone assessments.

1.4.6 ROMANS

The National Park Service (NPS), CDPHE/APCD and others have initiated the Rocky Mountain Atmospheric Nitrogen and Sulfur Study (ROMANS) to study nitrogen deposition and potential mitigation scenarios at Rocky Mountains National Park (RMNP). The Rocky Mountain Initiative includes data collection, data analysis, modeling and the development of a nitrogen deposition reduction plan. Much of the analysis of ROMANS was for the 2006 period that corresponds with the Denver 8-hour ozone modeling period that has direct relevance to the Denver ozone modeling. Details on the ROMANS study can be found at:

- http://www.cdphe.state.co.us/ap/rmnp.html

1.5 Overview of Modeling Approach

The Denver 8-Hour ozone SIP modeling includes emissions, meteorological and ozone simulations using a nested 36/12/4 km grid with the 4-km grid focused on the state of Colorado including the DMA and vicinity.

1.5.1 Ozone Episode Selection

Episode selection is an important component of an 8-hour ozone attainment demonstration. EPA guidance recommends that at least 10 days be used to project 8-hour ozone Design Values at each critical monitor, with 5 days being an absolute minimum.

1.5.1.1 EPA Guidance for Episode Selection

EPA's current guidance on 8-hour ozone modeling (EPA, 2007) identifies specific criteria to consider when selecting one or more episodes for use in demonstrating attainment of the 8-hour ozone National Ambient Air Quality Standard (NAAQS). This guidance builds off the 1-hour ozone modeling guidance (EPA, 1991) in selecting multiple episodes representing diverse meteorological conditions that result in ozone exceedances in the region under study:

- A variety of meteorological conditions should be covered, this includes the types of meteorological conditions that produce 8-hour ozone exceedances in the DMA and vicinity;
- To the extent possible, the modeling data base should include days for which extensive data bases (i.e. beyond routine aerometric and emissions monitoring) are available;
- Sufficient days should be available such that relative response factors (RRFs) can be based on several (i.e., $\geq$ 10) days with at least 5 days being the absolute minimum; and
- If possible and appropriate, modeling for an entire ozone season is recommended.

EPA also lists several "other considerations" to bear in mind when choosing potential 8-hour ozone episodes including:

- Choose periods which have already been modeled;
- Choose periods which are drawn from the years upon which the current Design Values are based;
- Include weekend days among those chosen; and
- Choose modeling periods that meet as many episode selection criteria as possible in the maximum number of nonattainment areas as possible.

1.5.1.2 Selection of Denver 8-Hour Ozone Modeling Period

The June through July 2006 period was selected for the Denver 8-hour ozone SIP modeling. Section 3 describes the rationale for selecting this modeling period with the main reasons being:

- It is included within the 2005-2007 three-year period which Denver's nonattainment status was based;
- Includes 8-hour ozone exceedance days at all the key high ozone monitors in the DMA; and
- Includes all exceedance days and most high ozone days in the DMA from 2006, which was the summer with the highest number of high 8-hour ozone days from the 2005-2007 period.

1.5.2 Model Selection

Details on the rationale for model selection are provided in Section 2. The MM5 prognostic meteorological model was selected for the Denver ozone modeling using a 36/12/4 km resolution grid, but with the 4-km grid covering most of Colorado. Emissions modeling will be performed using the SMOKE emissions model for most source categories, but with the CONCEPT emissions model used for on-road mobile sources in the DMA to take advantage of the detailed traffic information available and the MEGAN model used for biogenic emissions. The CAMx photochemical grid model, which supports two-way grid nesting and subgrid-scale Plume-in-Grid, will also be used. This is the same SMOKE/MM5/CAMx modeling system used in many recent ozone studies including FCAQTF and BLM EISs and is similar to the EPS3/MM5/CAMx modeling system used in the Denver 8-hour ozone EAC SIP modeling performed for 2002.

1.5.3 Emissions Input Preparation and QA/QC

Quality assurance (QA) and quality control (QC) of the emissions datasets are some of the most critical steps in performing air quality modeling studies. Because emissions processing is tedious, time consuming and involves complex manipulation of many different types of large databases, rigorous QA measures are a necessity to prevent errors in emissions processing from occurring. The Denver 8-Hour ozone modeling study will perform a multistep emissions QA/QC approach. This includes the initial emissions QA/QC by the CDPHE/APCD of their emissions for the DMA and surrounding areas, as well as QA/QC by the CDPHE/APCD and the modeling team as the dataset is processed and made available for modeling. This multi-step process with separate groups involved in the QA/QC of the emissions is designed to detect and correct errors prior to the air quality model simulations.

QA/QC performed as part of the emissions processing includes:

EPA Input Screening Error Checking Algorithms: Although the SMOKE emissions model is the primary tool used for emissions processing contains internal error checking and flagging, some additional input error checking algorithms, like those used with the EMS and EPS emission models, may be considered to screen the data and identify potential emission input errors. Additionally, EPA has issued a revised stack QA and augmentation procedures memorandum that will be used to identify and augment any outlying stacks.

SMOKE Error Messages: SMOKE provides various cautionary or warning messages during the emissions processing. The SMOKE output will be reviewed for error messages. An archive of the log files will be maintained so that the error messages can be reviewed at a later date if necessary.

SMOKE Emissions Summaries: QA functions built into the SMOKE processing system will be used to provide summaries of processed emissions as daily totals according to species, source category and county and state boundaries. These summaries will then be compared with summary data prepared for the pre-processed emissions, e.g., state and county totals for emissions from the augmented emissions data.

CONCEPT QA/QC: The CONCEPT model that will be used for generating the on-road mobile source emissions in the DMA was designed to be an open and transparent emissions modeling so has extensive QA/QC and error messaging system that will be used to QA this portion of the inventory.

MEGAN QA/QC: The MEGAN biogenic emissions model also includes error messages and warnings that need to be examined as part of the QA/QC of the biogenic emissions model. One of the most important components of the QA/QC of the biogenic emissions is assuring that proper land use data are input and that the MM5 surface temperatures are sufficiently accurate and that cloud information is represented correctly.

After the CAMx-ready emission inputs have been prepared, additional emissions QA/QC will be performed as appropriate, such as:

Spatial Summary: Sum the emissions for all 24 hours to prepare plots showing the spatial distribution of daily total emissions using the Package for Analysis and Visualization for Environmental (PAVE) data (available from www.cmascenter.org). In our base case simulations these plots will be presented as tons per day. Typically emission categories are processed using 5 streams of modeling: biogenic, on-road mobile, non-road mobile, other low-level anthropogenic and point sources (fires are also analyzed separately when available). If possible, separate spatial QA plots will be generated for low-level and elevated point sources. The objective of this step is to identify errors in the spatial distribution of emissions.

Short Term Temporal Summary: The total domain emissions for each hour will be accumulated and time series plots prepared by source category that display the diurnal variation in total hourly emissions. The objective of this step is to identify errors in temporal profiles.

Control Strategy Spatial Displays: Spatial summary plots of the daily total emissions differences between a future-year scenarios and base case emissions scenarios will be generated. These plots can be used to immediately identify a problem in a control strategy. For example, if a state's NOx emissions control strategy is being analyzed and there are changes in emissions for other pollutants or for NOx outside of the DMA, problems in emissions processing can be identified prior to the air quality model simulation.

The emissions QA/QC displays will be made available to study participants for review.

1.5.4 Meteorology Input Preparation and QA/QC

MM5 meteorological modeling of the selected modeling period will include QA/QC and evaluation of the meteorological fields. In addition, the modeling team will also perform QA/QC of the meteorological data to assure that it has been transferred correctly, to obtain an assessment of the quality of the data, and to assist in the interpretation of the air quality modeling results.

The modeling team will perform the following QA/QC of the MM5 meteorological fields developed for the study:

- Analyses of the various observational input and evaluation data sets to assure that they have been transferred correctly;
- Verification that correct configuration and science options are used in compiling and running each module in the MM5 modeling systems (TERRAIN, REGRID, RAWINS, INTERPF, etc.);
- Evaluation of the MM5 fields using the METSTAT program and the comparison of model performance statistics against performance benchmarks (see for example the WRAP MM5 evaluation at:
    - http://pah.cert.ucr.edu/aqm/308/reports/mm5/DrftFnl_2002MM5_FinalWRAP_Eval.pdf
- Evaluation of upper-air MM5 meteorological estimates by comparison to upper-air observations and satellite images;
- Evaluation of MM5 precipitation patterns and intensity against radar and rain-gauge analyses available from the Climatic Prediction Center;
- Comparison of the Denver MM5 simulation performance with those generated for the Denver EAC SIP and by WRAP and others;
- Generation of the CAMx-ready inputs with the MM5CAMx processor, and review of summary statistics generated by that program; and
- Backup and archiving of critical model input/output data.

1.5.5 Air Quality Modeling Input Preparation and QA/QC

Key aspects of QA for the CAMx input and output data include the following:

- Verification that correct configuration and science options are used in compiling and running each module in the CAMx modeling systems, where these include the MM5CAMx, TUV, landuse, and initial/boundary condition processors;
- Evaluation of CAMx results to verify that model output is reasonable and consistent with general expectations;
- Processing and QA of ambient monitoring data for use in the model performance evaluation;
- Evaluation of the CAMx results against concurrent observations and various other CAMx simulations;
- Backup and archiving of critical model input data.

The most critical elements for CAMx simulations are the QA/QC of the meteorological and emissions input files, which are discussed above, and the model performance evaluation. The major QA issue specifically associated with the air quality model simulations is verification that the correct science options were specified in the model itself and that the correct input files were used when running the model. This is accomplished to having multiple team members review the job script and job control file for each CAMx run prior to executing the program. Selected staff from ENVIRON and Alpine will be charged with reviewing each others CAMx simulation control files to assure the proper options and inputs are selected.

The modeling team will also perform a post-processing QA of the CAMx output files similar to that described for the emissions processing. Animated graphic files will be generated using PAVE that can be viewed to search for unexpected patterns in the CAMx output files. In the case of model sensitivity studies, the animated graphic files will be prepared as difference plots for the sensitivity case minus the base case. Often, viewing the animations can discover errors in the emissions inputs. Finally, daily maximum 1-hour and 8-hour ozone plots with superimposed observations will be produced for each day of the CAMx simulations. This will provide a summary that can be useful for quickly comparing various model simulations.

The Model Performance Evaluation (MPE) is a multi-step process using several different techniques:

> ENVIRON Analysis Tools: ENVIRON has developed ozone performance statistical techniques, “Soccer Plots”, time series plots, spatial maps and other summary plots that displays model performance across networks, episodes, species, models and sensitivity tests and compare them against performance goals. These tools can interface with Excel® to generate scatter plots and time series plots. It can also interface with SURFER® to generate spatial maps of model performance. ENVIRON has also developed software to generate 8-hour performance metrics and displays as recommended in EPA’s preliminary draft 8-hour ozone modeling guidance (EPA, 1999) that analyze predicted and observed daily maximum 8-hour ozone concentrations near each monitor.
>
> UCR Analysis Tools: The University of California at Riverside (UCR) has developed Analysis Tools that are used extensively in the CENRAP, VISTAS, and WRAP regional haze studies. Graphics are automatically generated using GNUPLOT that generates: (a) tabular statistical measures; (b) time Series Plots; and (c) scatter Plots by all sites and all days, all days for one site, and all sites for one day.

The evaluation of the CAMx base case simulations will use the appropriate analysis tools listed above to take advantage of their different descriptive and complimentary nature. The use of multiple model evaluation tools is also a useful QA/QC procedure to assure that errors are not introduced in the model evaluation process. Statistical performance measures for ozone, ozone precursors, and products species will be calculated to the extent allowed by the Denver ambient monitoring network database.

1.5.6 Proposed Model Performance Goals

The issue of model performance goals for 8-hour ozone concentrations is an area of ongoing research and debate. For 1-hour ozone modeling, EPA has established performance goals for unpaired peak performance, mean normalized bias (MNB) and mean normalized gross error (MNGE) of $<\pm 20\%$, $<\pm 15\%$ and $<35\%$, respectively (EPA, 1991). The EPA 8-hour ozone modeling guidance stresses performing corroborative and confirmatory analysis to assure that the model is working correctly (EPA, 2007). EPA's draft 8-hour ozone modeling guidance included comparisons of predicted and observed daily maximum ozone concentrations near the monitor with a $<\pm 20\%$ performance goal (EPA, 1999), however this goal was dropped from the final guidance (EPA, 2007). It may still be a useful performance metric and it was used in the Denver EAC SIP modeling. In evaluating the ozone and precursor model performance for the Denver 8-hour ozone modeling, many performance measures and displays will be used to elucidate model performance and maximize the probability of uncovering potential problems that can be corrected in the final runs.

1.5.7 Diagnostic and Sensitivity Studies

Rarely does a modeling team find that the first simulation satisfactorily meets all (or even most) model performance expectations. Indeed, our experience has been that initial simulations that "look very good", usually do so as the result of compensating errors. The norm is to engage in a logical, documented process of model performance improvement wherein a variety of diagnostic probing tools and sensitivity testing methods are used to identify, analyze, and then attempt to remove the causes of inadequate model performance. This is invariably one of the most technically challenging and time consuming phase of a modeling study. Due to the complex flows associated with the Denver Front Range meteorology, the CAMx model base case simulations will present some performance challenges that may necessitate focused diagnostic and sensitivity testing in order for them to be resolved. Below we identify the types of diagnostic and sensitivity testing methods that might be employed in diagnosing inadequate model performance and devising appropriate methods for improving the model response.

1.5.7.1 Traditional Sensitivity Testing

Model sensitivity experiments are useful in three distinct phases or "levels" of an air quality modeling study and all will be used as appropriate in the Denver ozone modeling. These levels are:

Level I:	Model algorithm evaluation and configuration testing;
Level II:	Model performance testing, uncertainty analysis and compensatory error diagnosis; and
Level III:	Investigation of model output response (e.g., ozone, aerosol, deposition) to changes in precursors as part of emissions control scenario analyses.

Most of the Level I sensitivity tests with CAMx have already been completed by the model developers (e.g., see www.camx.com) and others (e.g., the RPOs). However, given the open community nature of the CAMx model, the frequent science updates to the model and supporting databases, it is possible that some additional configuration sensitivity testing will be necessary.

Potential Level II sensitivity analyses might be helpful in accomplishing the following tasks:

- To reveal internal inconsistencies in the model;
- To provide a basis for compensatory error analysis;
- To reveal the parameters (or inputs) that dominate (or do not dominate) the model's operation;
- To reveal propagation of errors through the model; and
- To provide guidance for model refinement and data collection programs.

At this time, it is not possible to identify one or more Level II sensitivity runs that might be needed to establish a reliable CAMx base case. The merits of performing Level II sensitivity testing will depend upon whether performance problems are encountered in the operational evaluation. Also, the number of tests possible, should performance difficulties arise, will be limited by resources and schedule. Thus, at this juncture, one cannot be overly prescriptive on the number and emphasis of sensitivity runs that may ultimately be desirable. However, from past experience with CMAQ, CAMx, UAM and other models, it is possible to identify examples of sensitivity runs that could be useful in model performance improvement exercises with the CAMx Denver modeling databases. These include:

- Alternative meteorological realizations of the modeling period;
- Alternative vertical mixing rates and minimum vertical diffusion coefficient;
- Alternative (GloBEIS) and for modified biogenic emissions estimates;
- Modified on-road motor vehicle emissions;
- Modified air quality model vertical grid structure;
- Modified boundary conditions;
- Modified fire emissions; and
- Modified EGU emissions.

If desired, Process Analysis outputs can be included in these Level II diagnostic sensitivity simulations in order to provide insight into why the model responds in a particular way to each input modification. Other "Probing Tools" available in CAMx such as the Decoupled Direct Method (DDM) and Ozone Source Apportionment Technology (OSAT) may also be useful diagnostic tools to identify model performance issues. Again, the number, complexity, and importance of these types of traditional sensitivity simulations can only be determined once the initial CAMx base case simulations are executed.

Level III sensitivity analyses have two main purposes. First, they facilitate the emissions control scenario identification and evaluation processes. Today, four complimentary sensitivity "Probing Tools" can be used in the CAMx photochemical model:

- Traditional or "brute force" testing;
- The Decoupled Direct Method (DDM);
- Ozone Source Apportionment Technology (OSAT); and
- Process Analysis (PA).

Each method has its strengths and weaknesses and they will be employed where needed and as resources are available. The second purpose of Level III sensitivity analyses is to help quantify the estimated reliability of the air quality model in simulating the atmosphere's response to significant emissions changes.

Based on experience in other regional studies, examples of Level III annual sensitivity runs for Denver ozone analysis include:

- Ozone sensitivities to total VOC, NOx, CO and other emissions;
- Ozone sensitivity to on-road and non-road mobile VOC and NOx emissions;
- Ozone sensitivities to elevated point source NOx emissions;
- Ozone sensitivity to emissions due to oil and gas production; and
- Ozone sensitivity to NOx and VOC emissions from other specific source categories.

The need to perform sensitivity experimentation (Levels I, II, or III) will depend on the outcome of the initial Denver ozone operational performance evaluations. If such a need arises, the ability to actually carry out selected sensitivity and/or diagnostic experiments will hinge on the availability of resources and sufficient time to carry out the analyses. Clearly, selection of the specific analysis method will depend upon the nature of the technical question(s) being addressed at the time.

1.5.7.2 Diagnostic Tests

A rich variety of diagnostic probing tools are available for investigating model performance issues and devising appropriate means for improving the model and/or its inputs. In the previous section we introduced the suite of "Probing Tools" available for use in the CAMx modeling system. Where the need exists (i.e., if performance problems are encountered) and assuming the Denver modeling study elects to use probing tool applications, these techniques could be employed as appropriate to assist in the model performance improvement efforts associated with the Denver ozone base case development. At this time the study has not allocated resources for applying the probing tools for the 2006 base case to help diagnose model performance. However, there are resources allocated for ozone source apportionment modeling of the 2010 future-year.

Below we describe an additional diagnostic method – indicator species and species ratios – that is potentially useful not only in model performance improvement activities but also in judging the models reliability in estimating the impacts on air quality from future emissions. If, during the conducting of the Denver ozone simulations the application of indicator species and species ratio techniques would be beneficial to the study, it would be explored for inclusion in the study.

Beginning in the mid 1990s, considerable interest arose in the calculation of indicator species and species ratios as a means of diagnosing photochemical model performance and in assessing model credibility in estimating the effects of emissions changes. Major contributions to the development and refinement of this general diagnostic method over the past decade have been made many scientists including Milford et al., (1994), Sillman (1995, 1999), Sillman et al., (1997), Blanchard (2000), Blanchard and Fairley (2001), and Arnold et al., (2003).

Recent analytical and numerical modeling studies have demonstrated how the use of ambient data and indicator species ratios can be used to corroborate the future year control strategy estimates of Eulerian air quality models. Blanchard et al., (1999), for example used data from environmental (i.e., smog) chambers and photochemical models to devise a method for evaluating the 1-hour ozone predictions of models due to changes in precursor NOx and VOC emissions. Reynolds et al., (2003) followed up this analysis, augmented with process analysis, to assess the reliability of SAQM photochemical model estimate of 8-hour ozone to precursor emissions cutbacks. These researchers used three indicator ratios (or diagnostic "probes") to quantify the model's response to input changes:

- The ozone response surface probe [O3/NOx];
- The chemical aging probe [NOz/NOy]; and
- The ozone production efficiency probe [O3/NOz].

By closely examining the CMAQ's response to key input changes, properly focused in time and spatial location, Arnold and co-workers (2003) were able to show not only good agreement with measurements but also convincingly demonstrated the utility of the method for diagnosing model performance in a variety of ways.

1.5.8 Weight of Evidence Analyses

EPA's guidance recommends three general types of "weight of evidence" analyses in support of the attainment demonstration: (a) use of air quality model output, (b) examination of air quality and emissions trends, and (c) the use of corroborative modeling such as observation-based (OBM) or observation-driven (OBD) models. Use of these methods in conjunction with the CAMx modeling could significantly strengthen the credibility and reliability of the modeling available to the states for their subsequent use. The exact details of the weight of evidence (WOE) analyses must wait until the Denver ozone modeling study evolves further. It is premature to prescribe which, if any of the WOE analyses would be performed since both the model's level of performance for the Denver ozone modeling time and the level of the future-year projected 8-hour ozone Design Values are not known at this time. EPA requires a WOE analysis if the projected maximum future-year 8-hour ozone Design Values lies between 82 and 87 ppb (EPA, 2007). We believe it is always a good idea to perform WOE analysis to corroborate the modeled attainment demonstration. Many of the WOE analyses are independent of the photochemical modeling being conducted by the study team and can potentially be performed by the project sponsors or interested stakeholders. Below are thoughts regarding what would likely be considered as part of the WOE analyses.

Use of Emissions and Air Quality Trends: Emissions and air quality trend analysis is always an important component of a WOE analysis. When combined with meteorological analysis of the yearly ozone formation potential, it can be used to determine whether actual trends can corroborate the model projected determination of whether future-year air quality goals are achieved.

Use of Corroborative Observational Modeling: While regulatory modeling studies for ozone attainment demonstrations have traditionally relied upon photochemical models to evaluate ozone control strategies, there has recently been growing emphasis on the use of data-driven models to corroborate the findings of air quality models. As noted, EPA's guidance (EPA, 2007) now encourages the use of such observation-based or observation-driven models (OBMs/ODMs). The merits of using these techniques will be considered as supportive weight of evidence. While the OBD/OBM models cannot predict future year air quality levels, they do provide useful corroborative information on the extent to which ozone formation in specific subregions may be VOC-limited or NOx-limited, for example. Information of this type, together with results of DDM, PA and OSAT as well as traditional "brute-force" sensitivity simulations, can be extremely helpful in postulating emissions control scenarios since it helps focus on which pollutant(s) to control.

Other WOE Analysis: EPA's 8-hour ozone guidance (EPA, 2007) lists additional analysis that can be performed as part of the WOE including analysis of other studies, use of alternative models and the calculations of alternative model statistics. The use of all of these other techniques will be explored as appropriate.

1.5.9 Assessing Model Reliability in Estimating the Effects of Emissions Changes

EPA identifies three methods (e.g., EPA, 2001, pg. 228) potentially useful in quantifying a model's reliability in predicting air quality response to changes in model inputs, e.g., emissions. These include:

- Examination of conditions for which substantial changes in (accurately estimated) emissions occur;
- Retrospective modeling, that is, modeling before and after historical significant changes in emissions to assess whether the observed air pollution changes are adequately simulated; and
- Use of predicted and observed ratios of "chemical indicator species".

We note that in some urban-scale analyses, the use of weekday/weekend information has been helpful in assessing the model's response to emissions changes. Such analysis should be examined to determine whether it is appropriate for the Denver area.

The use of indicator species and ratios offers some promise, and was described earlier in Section 1.5.7.2. The first two methods have actually been considered for over 15 years and were the subject of intensive investigations in the early 1990s in Southern California in studies sponsored by the South Coast Air Quality Management District (Tesche, 1991) and the American Petroleum Institute (Reynolds et al., 1996). To date, neither method has proven useful largely because of the great difficulty in developing historical emissions inventories of sufficient quality to make such an analysis credible and the difficulties in removing the influences of different meteorological conditions such that the modeling signal reflects only the model's response to emissions changes. It is difficult enough to construct reliable emissions inventories using today's modeling technology let alone construct retrospective inventories 5-10 years ago prior to the implementation of significant emissions control programs, major land use changes and widespread adoption of Continuous Emissions Monitors.

The 2004 Denver 8-hour EAC SIP modeling offers a relevant example a retrospective type analysis of model performance. The Denver EAC SIP CAMx modeling of the summer of 2002 projected that the current (2001-2003) observed maximum 8-hour ozone DV of 87 ppb at the Rocky Flats North (RFNO) monitor would be 85 ppb in 2007. With the conclusion of the summer 2007 ozone season, the measured 8-hour ozone DV based on the 2005-2007 period at RFNO is in fact also 85 ppb.

1.5.10 Future Year Control Strategy Modeling

Future-year modeling for ozone will be performed for 2010. The Denver area is expected to be designated as a Marginal 8-hour ozone nonattainment area by EPA on November 20, 2007 under Subpart 2 of the Clean Air Act Amendments (CAAA).

1.5.11 Future Year Ozone Attainment Demonstration

The Denver modeling results will be used to demonstrate attainment of the 8-hour ozone NAAQS. The procedures to be used to demonstrate attainment of the ozone NAAQS will follow EPA guidance. Guidance procedures for demonstrating attainment of the 8-hour ozone standard has been finalized (EPA, 2007). These procedures use the modeling results in a relative fashion to scale the observed 8-hour ozone Design Values using Relative Reduction Factors (RRFs). RRFs are the ratio of the future-year to current-year modeling results and are used to scale the current-year 8-hour ozone Design Values to project future-year Design Values that are compared against the 8-hour ozone NAAQS to determine whether attainment has been demonstrated. EPA has developed the Modeled Attainment Test Software (MATS) tool that includes the EPA guidance 8-hour ozone DV projection techniques. Section 8 of this Protocol provides more details on the 8-hour ozone attainment demonstration modeling approach and details on EPA's new MATS tool can be found at:

- http://www.epa.gov/scram001/modelingapps_mats.htm

1.6 Project Participants and Contacts

The Denver Regional Air Quality Council (RAQC) and Colorado Department of Public Health and the Environment (CDPHE) Air Pollution Control Division (APCD) are the lead agencies in the development of the Denver 8-hour ozone SIP. They will work closely with other local agencies, including the Denver Regional Council of Governments (DRCOG) and Colorado Department of Transportation (CDOT), and EPA Region 8 in the SIP development, including the sharing of interim results as they become available. The Denver RAQC has contracted with a modeling team of ENVIRON International Corporation (ENVIRON) and Alpine Geophysics, LLC (Alpine) to perform the Denver 8-hour attainment demonstration modeling under the direction and with assistance from the RAQC and CDPHE/APCD. RAQC/APCD will also work with local agencies and stakeholders in the Denver SIP development, where stakeholders include environmental groups and industry. Key participants in the Denver 8-hour ozone study and their contact information are provided in Table 1-1.

Table 1-1. Key participants and contact information for the Denver 8-hour ozone attainment demonstration modeling study.

Organization	Individual(s) [Roll]	Address	Contact Numbers
U.S. EPA Region 8			
	Mr. Kevin Golden [EPA Contact]	Regional Meteorologist EPA Region VIII Denver, CO	bus: (303) 312-6442 fax: (303) 312-6064 e-mail: golden.Kevin@epa.gov
Regional Air Quality Council			
	Mr. Kenneth Lloyd	Executive Director 1445 Market Street, Suite 260 Denver, CO 80202	bus: (303) 629-5450 fax: (303) 629-5822 e-mail: klloyd@raqc.org
	Mr. Gerald Dilley [RAQC Project Manager]	Technical Program Manager 1445 Market Street, Suite 260 Denver, CO 80202	bus: (303) 629-5450, ext. 240 fax: (303) 629-5822 e-mail: jdilley@raqc.org
Colorado Department of Public Health and Environment Air Pollution Control Division			
	Mr. Kevin Briggs [APCD Modeling]	Air Pollution Control Division 4300 Cherry Creek Dr. South Denver, CO 80222	bus: (303) 692-3222 fax: (303) 782-5493 e-mail: krbriggs@smtpgate.dphe.state.co.us
	Mr. Dale Wells [APCD Emissions]	Air Pollution Control Division 4300 Cherry Creek Dr. South Denver, CO 80222	bus: (303) 692-3237 fax: (303) 782-5493 e-mail: DMWELLS@SMTPGATE.DPHE.STATE.CO.US
Colorado Department of Transportation (CDOT)			
	Ms. Gail Hoffman [MPO and Regional Planner]	4201 E. Arkansas Shumate Building Denver, CO 80222-3406	bus: (303) 757-9700 fax: (303) 757-9727 e-mail: Gail.Hoffman@dot.state.co.us
Denver Regional Council of Governments (DRCOG)			
	Mr. Eric Sabina	1290 Broadway, Suite 700 Denver, CO 80203-5606	bus: (303) 480-6789 fax: (303) 480-6790 e-mail: esabina@drcog.org
Contractors (modeling team)			
ENVIRON International Corporation	Mr. Ralph Morris [Project Manager and Co-Principal Investigator]	Managing Principal 773 San Marin Dr., Suite 2115 Novato, CA 94998	bus: (415) 899-0708 fax: (415) 899-0707 e-mail: rmorris@environcorp.com
Alpine Geophysics, LLC	Mr. Dennis McNally [Co-Principal Investigator]	Senior Scientist 7341 Poppy Way Arvada, CO 80007	bus: (303) 421- 4221 fax: (303) 421- 9553 e-mail: dem@alpinegeophysics.com

1.7 Communication

Frequent communication between the RAQC/APCD and EPA, and the modeling team as needed, is anticipated. These communications will include e-mails, conference calls and face-to-face meetings. The RAQC/APCD envisions that EPA and others will review interim products as they become available so that comments can be received during the study to allow for corrective action as necessary. These interim deliverables would include, but not be limited to, preliminary MM5 evaluation, preliminary current and future-year emissions assumptions and results, preliminary CAMx model performance evaluation and preliminary 8-hour ozone projections.

1.8 Schedule

Table 1-2 lists the schedule for key deliverables under the Denver 8-hour ozone modeling study. We intend to develop a fast track preliminary base case inventory for the June-July 2006 period by December 2007. Consequently we will rely on existing information and use the SMOKE emissions model for all anthropogenic emission sources. A more refined base case inventory will be developed by February 2008 that will include detailed on-road mobile source emissions for the DMA using CONCEPT. The schedule is driven by the need to propose an 8-hour ozone SIP control plan to the Colorado Air Quality control commission by September 2008. These dates will be updated as the study evolves.

Table 1-2. Key deliverables and dates for the Denver 8-hour ozone attainment demonstration modeling study.

Deliverable (Type)	Date
Preliminary Draft Modeling Protocol (Report)	October 23, 2007
Modeling Protocol Meeting (PPT and Presentation)	October 25, 2007
Draft Modeling Protocol (Report)	October 31, 2007
Initial MM5 36/12/4 km Jun-Jul 2006 Simulation (Inputs)	November 30, 2007
Preliminary Fast Track 3612/4 km Emissions (Inputs)	December 19, 2007
MM5 Sensitivity Tests (Inputs)	January 17, 2008
Initial Run and Preliminary CAMx Sensitivity Tests (PPT)	January 24, 2008
Final MM5 Optimal Configuration Run (PPT)	February 15, 2008
Final 2006 36/12/4 km Actual Emissions Base Case (Inputs)	February 22, 2008
Final CAMx Sensitivity Tests (PPT)	February 29, 2008
Final 2006 36/12/4 km Typical Emissions Base Case (Inputs)	March 21, 2008
Final 2006 36/12/4 km Actual CAMx Base Case Simulation (PPT)	March 21, 2008
Summary Report on Sensitivity Modeling and MPE (Report)	April 18, 2008
2010 36/12/4 km Base Case Emissions (Inputs)	April 18, 2008
2010 CAMx Base Case Simulation and Ozone Projections (PPT)	April 30, 2008
2010 Ozone Source Apportionment Modeling Results (PPT)	May 23, 2008
2010 Emission Reductions Sensitivity Results (PPT)	June 13, 2008
2010 Control Strategy Modeling Results (PPT)	August 8, 2008
Summary Report on 2010 Modeling (Report)	August 22, 2008
Draft Denver SIP Air Quality Technical Support Document (Report)	September 12, 2008
Final Denver SIP Air Quality Technical Support Document (Report)	September 26, 2008*
2020 Emissions and CAMx Modeling Results (PPT)	September 30, 2008
Disk Drives with Model Inputs, Databases, Models and Key Model Outputs (Disks)	September 30, 2008

* Assumes comments on draft Air Quality TSD received within one week.
PPT=Power Point Presentation

2.0 MODEL SELECTION

This section introduces the models to be used in the Denver 8-hour ozone modeling study. The selection methodology presented in this chapter rigorously adheres to EPA's guidance for regulatory modeling in support of ozone attainment demonstrations (EPA, 2007). Unlike previous ozone modeling guidance, the agency now recommends that models be selected for SIP studies on a "case-by-case" basis with appropriate consideration being given to the candidate models':

- Technical formulation, capabilities and features;
- Pertinent peer-review and performance evaluation history;
- Public availability; and
- 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 as it did sixteen years ago (EPA, 1991). After identifying the models we believe are best suited to the requirements of the Denver 8-hour ozone SIP modeling study, the justification for their selection is discussed. The actual science configurations recommended for each model in this study are introduced in Chapter 5.

EPA's new guidance on model selection and justification requires a substantial effort to document the past evaluation studies, peer-reviews and application efforts associated with the models recommended for use. Many of the relevant citations are presented in the References section of this protocol.

2.1 Regulatory Context for Model Selection

A comprehensive modeling protocol for the Denver 8-hour ozone attainment demonstration study consists of many elements. Its main function is to serve as a means for planning and communicating how a modeled attainment demonstration will be performed *before* it occurs (EPA, 1999; 2007). The protocol guides the technical details of a modeling study and provides a formal framework within which the scientific assumptions, operational details, commitments and expectations of the various participants can be set forth explicitly and means for resolution of potential differences of technical and policy opinion can be worked out openly and within prescribed time and budget constraints.

The modeling protocols for regulatory applications all too often fall short of providing sufficient detail in the description of the modeling assumptions and procedures to be employed (Roth et al., 2005). They are seldom updated as the modeling program ensues, notwithstanding declarations that they are "living documents". Part of the reason for this is that resource and schedule limitations necessitate greater emphasis on performing the modeling studies satisfactorily and on time and in addressing unexpected challenges that invariably arise; refining the protocol becomes a lower priority. As the cognizant lead agencies, the RAQC/APCD have the responsibility for updating relevant portions of this chapter of the protocol as new information is gained relative to the suitability of the models recommended for use in the Denver 8-hour ozone modeling.

2.1.1 Summary of Recommended Models

To develop new 8-hour ozone modeling episodes for the Denver area, the following state-of-science regional meteorological, emissions and air quality models will be used. The science features of these models and the justification for their selection are given later in this section. For the Denver 8-hour ozone modeling, we propose to use the MM5/SMOKE-CONCEPT-MEGAN/CAMx modeling system. This is almost the same modeling system that is being used to address ozone issues in southwest Colorado and northwest New Mexico in the FCAQTF study, by the NPS to address nitrogen deposition at RMNP as part of ROMANS and in southwest Wyoming for several oil and gas development EISs, and is similar to the MM5/EPS3/CAMx modeling systems used in the Denver and several other recent 8-hour ozone EAC SIPs that have been approved by EPA (e.g., San Antonio, Austin, Tyler-Longview Texas; Tulsa and Oklahoma City, Oklahoma; San Juan New Mexico).

MM5: The Fifth Generation Pennsylvania State University (PSU) National Center for Atmospheric Research (NCAR) Mesoscale Model (MM5) is a nonhydrostatic, prognostic meteorological model routinely used for urban- and regional-scale photochemical, fine particulate, and regional haze regulatory modeling studies (Dudhia, 1993; Seaman, 2000). Developed in the 1970s, the MM5 modeling system maintains its status as a state-of-the-science model through enhancements provided by a broad user community worldwide (Stauffer and Seaman, 1990; Xiu and Pleim, 2000; Byun et al., 2005a,b). MM5 is used nearly exclusively for regulatory air quality applications in the U.S. In recent years, the modeling system has been successfully applied in continental scale annual simulations.

SMOKE: The Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system is an emissions modeling system that generates hourly gridded speciated emission inputs of mobile, non-road, area, point, fire and biogenic emission sources for photochemical grid models (Coats, 1995; Houyoux and Vukovich, 1999). As with most 'emissions models', SMOKE is principally an emission processing system and not a true emissions modeling system in which emissions estimates are simulated from 'first principles'. This means that, with the exception of mobile and biogenic sources, its purpose is to provide an efficient, modern tool for converting an existing base emissions inventory data into the hourly gridded speciated formatted emission files required by an air quality simulation model. SMOKE will be used to prepare emission inputs for non-road mobile, area, point and on-road mobile sources outside of the DMA.

CONCEPT: The Consolidated Community Emissions Processing Tool (CONCEPT) is a new emissions modeling system that will be used to generate on-road mobile source emissions covered by the link-based Travel Demand Model (TDM) activity data within the DMA. The CONCEPT on-road mobile source component can make full use of linked-based vehicle miles traveled (VMT) data including temporal and spatial variations in speeds and fleet distributions. Details on the CONCEPT emissions model including user's guides, codes and related documentation is available at:

- http://www.conceptmodel.org

MEGAN: Biogenic emissions would be modeled using the Model of Emissions of Gases and Aerosols from Nature (MEGAN). MEGAN is the latest biogenic emissions model developed by researchers from the National Center for Atmospheric Research (NCAR) incorporates the full range of ozone and PM precursor species (Guenther and Wiedinmyer, 2004). In addition, the latest version of MEGAN includes biogenic species not found in other biogenic emissions model that are used by the latest CAMx secondary organic aerosol (SOA) module. MEGAN is a fairly new biogenic emissions model so we would also generate biogenic emissions using the BEIS algorithms that have been used in SIP modeling that would be used in a sensitivity test. Details on the MEGAN biogenic emissions model can be found at:

- http://bai.acd.ucar.edu/Megan/
- http://acd.ucar.edu/~christin/megan1.0_userguide.pdf

CAMx: The Comprehensive Air quality Model with Extensions (CAMx) is a state-of-science "One-Atmosphere" photochemical grid model capable of addressing ozone, particulate matter (PM), visibility and acid deposition at regional scale for periods up to one year (ENVIRON, 2006). CAMx is a publicly available open-source computer modeling system for the integrated assessment of gaseous and particulate air pollution. Built on today's understanding that air quality issues are complex, interrelated, and reach beyond the urban scale, CAMx is designed to (a) simulate air quality over many geographic scales, (b) treat a wide variety of inert and chemically active pollutants including ozone, inorganic and organic $PM_{2.5}$ and PM_{10} and mercury and toxics, (c) provide source-receptor, sensitivity, and process analyses and (d) be computationally efficient and easy to use. The U.S. EPA has approved the use of CAMx for numerous ozone and PM State Implementation Plans throughout the U.S. (including the Denver 8-hour ozone EAC SIP), and has used this model to evaluate regional mitigation strategies including those for most recent regional rules (e.g., CAIR, NOx SIP Call, etc.).

2.2 Details of the Recommended Models

Further details of the models we propose for use in the Denver 8-hour ozone modeling effort are described below. More information on these models may be obtained from the WRAP, VISTAS, CENRAP, and other modeling protocols (Morris et al., 2004a,b; Tesche et al., 2005b) and the literature references cited therein.

2.2.1 The MM5 Meteorological Model

The non-hydrostatic MM5 model (Dudhia, 1993; Grell et al., 1994) is a three-dimensional, limited-area, primitive equation, prognostic model that has been used widely in regional air quality model applications (Seaman, 2000). The basic model has been under continuous development, improvement, testing and open peer-review for more than 20 years (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. The model is also capable of using a hydrostatic option, if desired, for coarse-grid applications.

MM5 uses a terrain-following non-dimensionalized pressure, or "sigma", 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 "one atmosphere" air-quality models using this coordinate (e.g., CMAQ and CAMx). MM5 fields can be easily used in other regional air quality models with different coordinate systems (e.g., CAMx) by performing a vertical interpolation, followed by a mass-conservation re-adjustment.

Distinct planetary boundary layer (PBL) parameterizations are available for air-quality applications, all of which represent sub-grid-scale turbulent fluxes of heat, moisture and momentum. These parameterizations employ various surface energy budget equations to estimate 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 either defined as functions of land-use for numerous categories via a look-up table, or are provided as input fields from various terrestrial and large-scale analysis datasets.

Initial and lateral boundary conditions are specified from mesoscale three-dimensional analyses developed at 3-hour intervals on the outermost grid mesh selected by the user. Additional surface fields are also available at three-hour intervals. A Cressman-based technique is used to include standard surface and radiosonde observations into the analyses to improve local mesoscale representations. 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 (Stauffer and Seaman, 1990, 1996; Seaman et al., 1992, 1995, 1996).

Results of detailed performance evaluations of the MM5 modeling system in regulatory air quality application studies have been widely reported in the literature (e.g., Emery et al., 1999; Tesche and McNally, 1996b, 1997c, 1999, 2001; Sistla et al., 2001;Nielsen-Gammon, et al., 2005; Olerud and Sims, 2004a,b) and many have involved comparisons with other prognostic models such as RAMS. The MM5 enjoys a far richer application history in regulatory modeling studies compared with RAMS or other models. Furthermore, in evaluations of these models in over 60 recent regional scale air quality application studies since 1995, it has generally been found that MM5 model tends to produce somewhat better photochemical model inputs than alternative models (Tesche et al., 2002).

2.2.2 The Emissions Modeling Systems

Emissions modeling for the Denver 8-hour ozone modeling will be conducted using three separate emissions models: MEGAN model for biogenic sources; CONCEPT model for on-road mobile sources in the DMA and SMOKE model for everything else.

2.2.2.1 SMOKE Emissions Modeling System

SMOKE will be used to perform the emissions modeling for non-road mobile, area and point source emissions as well as on-road mobile outside of the DMA. SMOKE has been available since 1996, and it has been used for emissions processing in a number of regional air quality modeling applications. In 1998 and 1999, SMOKE was redesigned and improved with the support of the U.S. Environmental Protection Agency (EPA), for use with EPA's Models-3/CMAQ (http://www.epa.gov/asmdnerl/models3) and is currently maintained and available from the CMAS center (http://www.cmascenter.org).

As an emissions processing system, SMOKE has far fewer 'science configuration' options compared with the MM5 and CAMx models. SMOKE will be configured using the same spatial and temporal allocation profiles as used in the WRAP and FCAQTF modeling, updated to local conditions as appropriate.

2.2.2.2 MEGAN Biogenic Emissions Model

MEGAN will be used to generate VOC and NOx emissions for the 36/12/4 km grid from biogenic emission sources. MEGAN generates biogenic emissions using land cover database of biomass type and density and hourly meteorological data. NCAR has prepared a global database of land use data for use with MEGAN, the MEGAN
Driving Variable Database (MDVD Version 2.1). Surface temperatures will come from the MM5 modeling.

2.2.2.3 CONCEPT Emissions Modeling

Although CONCEPT is a complete emissions modeling system for all source categories, we will just be using the on-road mobile source component. CONCEPT was developed by ENVIRON and Alpine Geophysics and designed to be an open transparent emissions modeling system. The on-road mobile of CONCEPT is the most advanced emissions treatment available making full use of link-based VMT data.

2.2.3 The CAMx Regional Photochemical Model

The Comprehensive Air quality Model with Extensions (CAMx) is a publicly available (www.camx.com) three-dimensional multi-scale photochemical/aerosol grid modeling system that is developed and maintained by ENVIRON International Corporation. CAMx was developed with all new code during the late 1990s using modern and modular coding practices. This has made the model an ideal platform to treat a variety of air quality issues including ozone, particulate matter (PM), visibility, acid deposition, and air toxics. The flexible CAMx framework has also made it a convenient and robust host model for the implementation of a variety of mass balance and sensitivity analysis techniques including Process Analysis (IRR, IPR, and CPA), Decoupled Direct Method (DDM), and the Ozone/PM Source Apportionment Technology (OSAT/PSAT). Designed originally to address multiscale ozone issues from the urban- to regional-scale, CAMx has been widely used in recent years by a variety regulatory agencies for 1-hour and 8-hour ozone SIP modeling studies. Key attributes of the CAMx model for simulating gas-phase chemistry include the following:

- Two-way grid nesting that supports multiple levels of fully interactive grid nesting (e.g., 36/12/4/1.33 km);
- CB05, CB4 or SAPRC99 chemical mechanisms;
- Two chemical solvers, the CAMx Chemical Mechanism Compiler (CMC) Fast Solver or the highly accurate Implicit Explicit Hybrid (IEH) solver;
- Multiple numerical algorithms for horizontal transport including the Piecewise Parabolic Method (PPM) and Bott advection solvers;
- Subgrid-scale Plume-in-Grid (PiG) algorithm to treat the near-source plume dynamics and chemistry from NOx, VOC SOx, and/or PM point source plumes;
- Ability to interface with a variety of meteorological models including the MM5, WRF and RAMS prognostic hydrostatic meteorological models and the CALMET diagnostic meteorological model (others also compatible);
- The Ozone Source Apportionment Technology (OSAT) and PM Source Apportionment Technology (PSAT) that identifies the ozone or PM contribution due to geographic source regions and source categories (e.g., mobile, point, biogenic, etc.); and
- The Decoupled Direct Method (DDM) sensitivity method is implemented for emissions and IC/BC to obtain first-order sensitivity coefficients for all gas-phase and particle-phase species.

Culminating from extensive model development efforts at ENVIRON and other participating groups, the CAMx Versions 4.5 will be released in 2007 as a truly "One-Atmosphere" model that rigorously integrates the gas-phase ozone chemistry with the simulation of primary and secondary fine and coarse aerosols. This extension of CAMx to treat PM involved the addition of several science modules to represent important physical processes for aerosols. Noteworthy among these are:

- Two separate treatments of PM: Mechanism 4 (CF) uses two static size sections and science modules comparable to CMAQ (e.g., RADM aqueous-phase chemistry and ISORROPIA equilibrium); and Mechanism 4 (CMU) uses a multi-section "full-science" approach using aerosol modules developed at Carnegie Mellon University (CMU).
- The size distribution in the CMU approach is represented using the Multi-component Aerosol Dynamics Model (MADM), which uses a sectional approach to represent the aerosol particle size distribution (Pilinis et al., 2000). MADM treats the effects of condensation/evaporation, coagulation and nucleation upon the particle size distribution.
- Inorganic aerosol thermodynamics can be represented using ISORROPIA (Nenes et al, 1998; 1999) equilibrium approach within MADM, or a fully dynamic or hybrid approach can also be used.
- Secondary organic aerosol thermodynamics are represented using the semi-volatile scheme of Strader and co-workers (1999).

- Aqueous-phase chemical reactions are modeled either using the RADM module (like CMAQ) or the Variable Size-Resolution Model (VRSM) of Fahey and Pandis (2001), which automatically determines whether water droplets can be represented by a single "bulk" droplet-size mode or whether it is necessary to use fine and coarse droplet-size modes to account for the different pH effects on sulfate formation.
- The PM Source Apportionment Technology (PSAT) "Probing Tool" can separately track PM source apportionment for SO4/NO3/NH4, SOA, Primary PM and Hg families of tracers.

In 2007 ENVIRON is releasing CAMx v4.5 that will be the most current version of CAMx available on the website (www.camx.com). Version 4.5 includes several improvements geared mainly toward improved PM simulations over earlier versions including updates to the SOA module to include SOA from isoprene and sesquiterpene emissions from the MEGAN biogenic emissions model.

2.3 Justification for Model Selection

2.3.1 MM5

The most commonly used prognostic meteorological models to support air quality modeling are the MM5 and the Regional Atmospheric Modeling System (RAMS). The new Weather Research Forecast (WRF) model shows promise as a meteorological driver for air quality models, but it needs further demonstration before it can be used in a regulatory modeling study. A number of recent studies inter-compare the theoretical formulations and operational features of the MM5 and RAMS models and evaluate their performance capabilities under a range of atmospheric conditions. 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. Consistent with these evaluation studies, the MM5 is recommended as the prognostic meteorological modeling component for the Denver ozone study for the following reasons:

- All of the available state-of-science regional photochemical models identified in EPA's 8-hour 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 recent scientific model inter-comparisons examining over sixty 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 CAIR, CAMR, SAMI, NARSTO, SARMAP, SCOS, SCAQS, VISTAS, MANE-VU, CENRAP, MRPO, and WRAP as well as in a number of urban-scale SIP applications (e.g., Pittsburgh, Cincinnati, San Juan, Kansas City, St. Louis, Denver, Tulsa, Houston, Dallas, Central California, Phoenix, Boise, etc.).

- While MM5 and RAMS meteorological models have been used for air quality modeling in different urban and regional-scale studies, in most regulatory ozone applications the MM5 model has been the preferred system.

2.3.2 Emissions Models

The MEGAN, CONCEPT and SMOKE emissions modeling systems are the recommended emissions models for the Denver 8-hour ozone modeling study for the following reasons:

- MEGAN is the latest biogenic emissions model and incorporates the latest scientific knowledge. It also includes biogenic precursor emissions to support the new SOA module in CAMx. It has been tested for a variety of applications including the FCAQTF .
- CONCEPT will be used for modeling on-road mobile sources. It is the most advanced link-based on-road emissions modeling system that has been extensively tested using 19 link-based networks in the Midwest as well as Las Vegas. This is in contrast to the SMOKE link-based module that has only been used once (by ENVIRON for the St. Louis 8-hour ozone SIP) which requires constant vehicle speeds and fleet mixes across all links.
- The SMOKE emissions model has been operational for over a decade and is fully supported by the EPA through the CMAS Center (www.cmascenter.org). It is the most computationally efficient of the emissions models and is being used by WRAP and the FCAQTF.

2.3.3 CAMx

During the NARSTO Critical Tropospheric Ozone Assessment, two major reviews of photochemical modeling were performed. Russell and Dennis (2000) compared the scientific and operational features of essentially all current recent Eulerian photochemical models in use up to that time. In parallel, Roth et al. (1998, 2005) reviewed more than twenty regulatory applications of photochemical models in the U.S. and Canada. From these reviews, and the modeling team’s experience with each of these models, we recommend CAMx as the ozone modeling tool for the Denver study for the following reasons:

- CAMx is a state-of-science “one-atmosphere” model;
- CAMx has undergone extensive successful testing by a variety of groups for nearly a decade.
- CAMx is unique among state-of-science “one-atmosphere” air quality models in its ability to offer ozone and particulate source apportionment technology (OSAT, PSAT), Process Analysis, and the DDM sensitivity analysis scheme.
- CAMx has been used extensively for numerous recent 8-hour ozone SIPs including Denver, Oklahoma, St. Louis, and areas in Texas and other regulatory modeling including the EPA to support for regulatory decision making (e.g., CAIR, NOx SIP Call, etc.).
- CAMx is a public-domain model, available free of charge, without restriction (www.camx.com).

2.4 Model Limitations

All mathematical models possess inherent limitations owing to the necessary simplifications and approximations made in formulating the governing equations, implementing them for numerical solution on fast computers, and in supplying them with input data sets and parameters that are themselves approximations of the full state of the atmosphere and emission processes. Below, we list the more important limitations of the various modeling systems to be employed in the Denver 8-hour ozone study.

2.4.1 MM5

In VISTAS (Morris et al., 2004a,b), four different configurations of the MM5 Land Soil Model (LSM) and Planetary Boundary Layer (PBL) were evaluated. Depending on the meteorological variable (e.g., winds, temperature, moisture) and location (e.g., mountains, coastal, east, west), different LSM_PBL configurations performed better. For VISTAS, the Pleim-Xiu PBL scheme (Xiu and Pleim, 2000) was selected because it was consistently the top performing configuration across the VISTAS domain. However, detailed research in Houston by UH/IMAQS (Byun et al., 2005a,b) have revealed that their modified MRF PBL scheme appears to better match the local meteorological conditions of their study region. The proper treatment of vertical turbulent mixing and the estimate of the PBL heights are among the important current science limitations in the model.

2.4.2 SMOKE

All emissions modeling systems have uncertainties and limitations. Foremost among these are the initial emissions estimates provided as input to the emissions models. However, even with exact emission estimates as inputs (an unlikely event) the emissions models still have numerous limitations just because of the shear volume of data that needs to be characterized and processed and the limited amount of data available to make the characterization:

Spatial Allocation: Emissions modeling system use surrogate distributions to spatially distribute county-level emissions. For example agricultural land use category would be used to spatially distribute agricultural equipment emissions, population may be used for a variety of home related emissions (e.g., home heating, aerosol sprays, etc.). The accuracy of these surrogate distributions will likely vary by source category.

Temporal Allocation: The allocation of annual average emissions to months and across the diurnal cycle use typical distributions by source category. The accuracy of these temporal allocations varies by source type within broader categories (e.g., heavy-duty diesel vs. light duty gas within the on-road category). They may also vary over different days. For example, a typical temporal distribution for a Sunday may be quite different on days when the Denver Broncos are in town.

Chemical Speciation: Emission models need to chemically speciate the VOC emissions into the photochemical mechanism (e.g., CB4) used in the photochemical grid model based on industrial codes. There are actually a limited number of speciation profiles and individual source tests have not been conducted for all different types of sources; consequently speciation profiles are assigned to "similar" sources that have source profile measurements.

Emission Projections: Projecting emissions introduce the largest layer of uncertainty. Emission projections include growing emissions from a current (e.g., 2006) to future (e.g., 2010 and 2020) year and then the application of any appropriate controls. Both of these steps are characterized by potentially huge limitations.

2.4.3 CAMx

Like all air quality models, there are a number of conceptual, physical, chemical, computational and operational challenges that CAMx model developers and the user community face to one extent or another. One current limitation is the treatment of vertical turbulent mixing where there are alternative means for estimating the time and space variation in turbulent mixing. Another common drawback of CAMx is the extensive emissions, meteorological and IC/BC inputs needed to operate the model. Treatment of clouds and wet deposition is an area of current research that needs to be updated. A practical limitation of CAMx is the computational requirements, including the need of significant disk space.

None of the current limitations identified in the MM5, SMOKE/CONCEPT/MEGAN and CAMx models render any of these models inappropriate for their use in this study, and are in fact common to all current models available for this type of application. However, such limitations need to be recognized and accounted for in the interpretation of the modeling results.

2.5 Model Input Requirements

Each of the modeling system components has significant data base requirements. These data needs fall into two categories: those required for model setup and operation, and those required for model evaluation and testing. Below, we identify the main input data base requirements for the meteorological, emissions, and air quality models. Details on the sources of the required data and how they will be used to construct model inputs are discussed in Chapter 5.

2.5.1 MM5

The databases required to set up, exercise, and evaluate the MM5 model consists of various fixed and variable inputs including: (a) topography, (b) vegetation type, (c) land use, (d) atmospheric data, (e) water temperature, (f) clouds and precipitation; and (g) multi-Scale FDDA data. Much of this data is available from the NCAR website.

2.5.2 Emissions

The databases required to set up and operate SMOKE for the Denver non-road, area and point source emissions modeling are as follows (a) area source emissions in IDA format, (b) non-road mobile source emissions in IDA format, (c) stationary point source emissions in IDA format, (d) CEM emissions, day specific, and (e) wildfire emissions, day specific. Also required are data files specific for temporal allocation, spatial allocation, and chemical speciation.

To operate the CONCEPT model for on-road mobile sources emissions in the DMA we need 2006, 2010 and 2020 link-based VMT data with temporal and spatial variations in speeds and fleet mix and MOBILE6 inputs for the three years and local fuel characteristics. We also need the fraction of counties covered by the TDM link-based data. For outside of the DMA we need county-level 2006, 2010 and 2020 VMT data and appropriate MOBILE6 inputs. We also need meteorological data, which would come from MM5.

For the MEGAN biogenic emissions modeling detailed land cover data is needed to characterize biomass type and density and hourly meteorological data (MM5).

2.5.3 CAMx

Major CAMx model inputs include: (a) three-dimensional hourly meteorological fields generated by MM5 via the MM5CAMx interface tool, (b) three-dimensional hourly emissions generated by SMOKE/CONCEPT/MEGAN, (c) initial conditions and boundary conditions (IC/BC), (d) photolysis rates look up table, (e) albedo/haze/ozone Column input file, and (f) land use.

2.6 Summary of Model Selection and Justification

In summary, the MM5, SMOKE/CONCEPT/MEGAN and CAMx regional models are recommended for use in the Denver 8-hour ozone modeling 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 8-hour ozone photochemical modeling study.

We conclude the model selection discussion by presenting in Tables 2-1 through 2-4 the six (6) criteria set forth in EPA's draft 8-hour modeling guidance (EPA, 2005a; 2007) 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 selected are indeed suitable candidates for this application. Tables 2-5 through 2-8 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 2-1 though 2-8 supports our recommendation that the MM5, SMOKE/CONCEPT/MEGAN and CAMx models are logical choices given the specific technical, regulatory, schedule and resource aspects of the Denver 8-hour ozone modeling study.

2.7 Availability of Model Codes, Analysis Tools and Related Software

The source codes, user's guides, analysis tools, documentation and related software for all models used in this study are publicly available. These models and their pre- and post-processor programs and test data bases may be obtained from the following websites:

MM5:	http://www.mmm.ucar.edu/mm5/overview.html
SMOKE:	http://www.cmascenter.org
CONCEPT:	http://www.conceptmodel.org
MEGAN:	http://bai.acd.ucar.edu/Megan/
CAMx:	http://www.camx.com

Table 2-1. Factors qualifying MM5 for use in the Denver 8-hour ozone modeling 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); Emery et al., (1999, 2001); Barchet and Dennis (1990); Tesche and McNally (1993e,f); Pielke and Pierce (1994); and Seaman (1995, 2000, 2005). 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, MM5 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 databases 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 “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 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 (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), 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. The MM5 model has been used extensively in the Denver and nearby areas for the EAC SIP, ROMANS study and FCAQTF modeling.
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 its 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 2-2. Factors qualifying SMOKE, CONCEPT and MEGAN emissions models for use in the Denver ozone modeling study.

Consideration	Qualification
The model has received scientific peer review.	A formal scientific review of the SMOKE modeling system has been continuous since its first release in 1996 that is now being performed as part of the CMAS Center operations (www.cmascenter.org). Numerous governmental, educational and private modeling groups in the U.S. and abroad have engaged in ongoing review, testing, and evaluation of the SMOKE model code as part of training, model set-up, exercise, and quality assurance activities. In particular, the RPOs have performed extensive testing and peer-review of the SMOKE modeling system and the CMAS Center conducts training on its use. The CONCEPT emissions model is in the process of undergoing a more detailed review. The on-road mobile source component of CONCEPT to be used in the Denver study has undergone detailed testing and scientific peer review using 19 link-based networks in the Midwest and Las Vegas. The MEGAN biogenic emissions model has undergone extensive testing and peer review since it was released in 2004. Scientists at ENVIRON and Alpine have reviewed the code.
The model can be demonstrated to be applicable to the problem on a theoretical basis.	The SMOKE and CONCEPT emissions modeling systems were 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. SMOKE and CONCEPT are two of the four state-of-science regional emissions models actively used in the U.S. and abroad (others are EMS and EPS). The features and capabilities of the SMOKE and CONCEPT modeling system are consistent with the application on a combined urban- and regional-scale, as required in the Denver modeling study. The MEGAN model represents the most up-to-date and advanced biogenic emissions modeling system available and is the only biogenic emissions model that provides sufficient information for the advanced SOA module in CAMx.
Date bases needed to perform the analysis are available and adequate.	Key input data bases to the SMOKE, CONCEPT and MEGAN emissions modeling systems (e.g., point, area, and motor-vehicle sources plus biogenic sources) are available from the CDPHE/APCD, EPA and WRAP. Model inputs will be prepared following published User's Guidelines, the development of the APCD, WRAP, CENRAP, and VISTAS regional inventories, and those used by EPA in the development of the CAIR modeling. The adequacy of the input data bases developed by these various sources will be assessed as part of the emissions 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 MOBILE6. Non-road mobile sources emissions are based on EPA's NONROAD model.
A protocol on methods and procedures to be followed has been established.	The protocol is outlined in this document. The SMOKE, CONCEPT and MEGAN emissions 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.	SMOKE, CONCEPT and MEGAN emission models are all in the public domain and can be downloaded from: SMOKE: http://www.cmascenter.org CONCEPT: http://www.conceptmodel.org MEGAN: http://bai.acd.ucar.edu/Megan/

Table 2-3 Factors qualifying CAMx as the photochemical grid model for use in the Denver ozone modeling study.

Consideration	Qualification
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 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 with CAMx are cited in the references section. 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 its 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. 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 2-4. Factors justifying MM5 as the meteorological model for the Denver ozone modeling study.

Consideration	Qualification
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 circulations over the Denver study area as well as other mesoscale features including convergence zones, cumulus convection, complex terrain effects and so on. The nested grid feature of MM5 will directly support the urban- to regional-scale nesting schemes in CAMx.
Availability, documentation and past performance should be satisfactory.	The MM5 modeling system is publicly available and has been regularly used in support of CAMx modeling studies across the country. It has also been successfully used for several air quality studies in the 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, numerous 8-hr ozone EAC studies (e.g., Denver/Northern Front Range EAC, the Kansas City/Missouri region). MM5 is the model used in all of the RPO studies currently being performed for Regional Haze. 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, 2005).
Relevant experience of available staff and contractors should be consistent with choice of a model.	The MM5 modeling will be performed by ENVIRON who are thoroughly knowledgeable of the use of the model for mesoscale research applications as well as in regulatory photochemical modeling studies.
Time and resource constraints may be considered.	Use of the MM5 model is consistent with the Denver 8-hour ozone SIP development schedule.
Consistency of the model with what was used in adjacent regional applications should be considered.	MM5 has been applied in several photochemical modeling studies (e.g., Denver EAC study, 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 Missouri, 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 ATMOS.

Table 2-5. Factors justifying SMOKE/CONCEPT/MEGAN as the emissions model for the Denver ozone modeling study.

Consideration	Qualification
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.	SMOKE/CONCEPT/MEGAN were designed for the preparation of detailed urban- and regional-scale photochemical modeling inventories such as is required for the Denver study. CONCEPT emissions model represents the most accurate and detailed representation of on-road mobile sources ever. MEGAN is the most current and accurate biogenic emissions model. SMOKE has been used extensively by the RPOs and others for numerous air quality studies.
Availability, documentation and past performance should be satisfactory.	SMOKE, CONCEPT, MEGAN and MOBILE6.2 are publicly available at no charge. One or more of these models have been successfully used in a variety of regional modeling studies including 1-hour ozone attainment studies, several 8-hour ozone EAC SIPs, OTAG, SAMI, the EPA NOx SIP Call, CAIR, CAMR and CAVR.
Relevant experience of available staff and contractors should be consistent with choice of a model.	The emissions modeling tasks for the Denver study will be performed by ENVIRON and Alpine who have substantial experience in using these models and are the developers of CONCEPT.
Time and resource constraints may be considered.	Use of the SMOKE, CONCEPT, MEGAN and MOBILE6.2 models is consistent with the Denver project schedule.
Consistency of the model with what was used in adjacent regional applications should be considered.	SMOKE, CONCEPT, MEGAN, and MOBILE6.2 models (or their predecessors) have been applied in several recent photochemical modeling studies in adjacent areas including the FCAQTF, WRAP, ROMANS and southwest Wyoming BLM EIS photochemical modeling.

Table 2-6. Factors justifying CAMx as the photochemical model for the Denver ozone modeling study.

Consideration	Qualification
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 1-hr and 8-hr ozone data and review of climatological data sets in Denver, the potential 8-hr ozone nonattainment problems in the region include both regional and local components and are usually strongly influenced by the complex meteorology of the Front Range 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 complex terrain circulations (e.g., upslope/downslope), convective circulations, vertical mixing and cloud processes. The process-analysis, ozone source apportionment, and direct decoupled sensitivity analysis algorithms (DDM) in CAMx can 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 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 for ozone has consistently been comparable to or better than that of other contemporary model such as the CMAQ, 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, who developed the CAMx model, and Alpine, who have extensive experience in its application.
Time and resource constraints may be considered.	Use of the CAMx model is consistent with the Denver 8-hour ozone project schedule.
Consistency of the model with what was used in adjacent regional applications should be considered.	CAMx has or is being applied in several recent nearby photochemical modeling studies including the Denver EAC SIP, FCAQTF, WRAP, ROMANS, and BLM EIS modeling.

3.0 EPISODE SELECTION

3.1 Overview of EPA Guidance

EPA 8-hour modeling guidance (EPA, 2007) contains recommendations for selecting modeling episodes, while also referencing EPA's 1-hour ozone modeling guidance for episode selection (EPA, 1991).

3.1.1 Primary Criteria

EPA's guidance on 8-hour ozone modeling (EPA, 2007) identifies specific criteria to consider when selecting one or more episodes for use in demonstrating attainment of the 8-hour ozone National Ambient Air Quality Standard (NAAQS). The 8-hour ozone guidance builds off the 1-hour ozone guidance in selecting multiple episodes representing diverse meteorological conditions that result in ozone exceedances in the region under study, and includes the following criteria:

- A variety of meteorological conditions should be covered, including the types of meteorological conditions that produce 8-hour ozone exceedances in the Denver area;
- Choose episodes having days with monitored 8-hour daily maximum ozone concentrations close to the observed fourth highest value;
- To the extent possible, the modeling data base should include days for which extensive data bases (i.e. beyond routine aerometric and emissions monitoring) are available; and
- Sufficient days should be available such that relative response factors (RRFs) can be based on several (i.e., $\geq$ 10) days with at least 5 days being the absolute minimum.

3.1.2 Secondary Criteria

EPA also lists several "other considerations" to bear in mind when choosing potential 8-hour ozone episodes including:

- Choose periods which have already been modeled;
- Choose periods that are drawn from the years upon which the current Design Values are based;
- Include weekend days among those chosen; and
- Choose modeling periods that meet as many episode selection criteria as possible in the maximum number of nonattainment areas as possible.

EPA suggests that modeling an entire summer ozone season would be a good way to assure that a variety of meteorological conditions are captured and that sufficient days are available to construct robust RRFs for the 8-hour ozone Design Value projections.

3.2 Selection of Denver 8-hour Ozone Modeling Episode(s)

Measured ozone air quality data in the Denver area from the 2002 to 2007 six year period were analyzed to determine an optimal modeling period for performing 8-hour ozone Design Value projections for the 2010 future-year.

3.2.1 Key Denver Ozone Monitors

Table 3-1 displays the fourth highest 8-hour ozone concentrations at monitors in the Denver area for the years 2005 through 2007 and the 2005-2007 8-hour ozone Design Values (DVs). Locations of these monitors are given in Figures 4-1e and 4-2 and Table 4-5. The Rocky Flats North (RFNO) monitor to the northwest of downtown Denver has a 2005-2007 8-hour ozone Design Value (DV) of 85 ppb that exceeds the ozone NAAQS (85 ppb or higher). Observations from this monitor are why EPA is expected to designate the Denver area as an ozone nonattainment area in November 2007. The next highest 8-hour ozone DV is 84 at the Chatfield (CHAT) site south of Denver followed by NREL (82 ppb) west of downtown Denver and South Boulder Creek site (SBC; 81 ppb) that is a little further northwest of downtown Denver than RFNO. Although it only has two years of monitoring data so a valid three-year 8-hour ozone Design Value cannot be constructed, the Fort Collins West (FTCW) site is also recording high ozone levels and the average of the fourth highest 8-hour ozone over two years (2006-2007) of monitoring is 86 ppb that exceeds the NAAQS. Thus any future ozone air quality planning should also consider the FTCW monitoring site in the analysis.

Table 3-1. Fourth highest daily maximum 8-hour ozone concentrations (ppm) at monitoring sites in the Denver area during 2005, 2006 and 2007 and 2005-2007 8-hour ozone Design Values.

Site Name	2005 4th Maximum 8-Hour Average Value (ppm)	2006 4th Maximum 8-Hour Average Value (ppm)	2007 (thru 8/31) 4th Maximum 8-Hour Average Value (ppm)	2005 - 2007 3-Year Average 4th Maximum Value (ppm)
Welby	0.073	0.069	0.070	0.070
Highland	0.080	0.081	0.075	0.078
S. Boulder Creek	0.076	0.082	0.085	0.081
Denver – CAMP	0.051	0.062	0.057	0.056
Carriage	0.074	0.072	0.076	0.074
Chatfield State Park	0.084	0.086	0.082	0.084
USAF Academy	0.077	0.072	0.071	0.073
Manitou Springs	0.075	0.076	0.072	0.074
Arvada	0.078	0.082	0.078	0.079
Welch	0.064	0.081	0.080	0.075
Rocky Flats North	0.077	0.090	0.090	**0.085**
NREL	0.079	0.083	0.085	0.082
Fort Collins – West	---	0.087	0.085	---
Fort Collins	0.076	0.078	0.069	0.074
Greeley – Weld Tower	0.078	0.082	0.074	0.073
Rocky Mountains NP	0.075	0.076	0.078*	0.076*

* RMNP 2007 data only through July 31, 2007

3.2.2 Episode Selection Approach

We focus our episode selection to periods that occurred over the last 6 years (2000-2007). Daily maximum 8-hour ozone concentrations were analyzed from May 1 to August 31 over these six years to determine the optimal period for 8-hour ozone modeling. There is a preference for modeling a more recent year to reflect current emission conditions including fleet turnover and the implementation of the EAC SIP control measures. Episodes that occur during the 2005-2007 period that determined whether Denver would be a nonattainment area will be preferred (although the Denver ozone nonattainment classification is based on the 2001-2003 DVs). There is also a preference to model an entire or most of one summer during which ozone exceedances and high ozone levels occurred at all of the key ozone monitors.

3.2.3 High Ozone Levels from 2002-2007

Figure 3-1 displays the number of days during each year from 2002-2007 that the highest daily maximum 8-hour ozone concentration at any monitor in the Denver area was greater than or equal to 70, 75 and 85 ppb. 2003 has the most 8-hour ozone exceedance days in the Denver area with 22, whereas 2004 and 2005 have the least number of 8-hour ozone exceedance days with 0 and 3, respectively. 2002, 2006 and 2007 all have the more typical nine 8-hour ozone exceedance days.

When performing 8-hour ozone projections, EPA guidance recommends using modeling results from at least 10 modeling days (with a minimum of 5 modeling days) with elevated ozone concentrations at each monitoring site (EPA, 2007). Initially, EPA recommends selecting modeling days for use in 8-hour ozone projections for days when the base case modeled ozone concentration near a monitor is 85 ppb or greater, but this threshold is allowed to be relaxed to as low as 70 ppb in order to increase the number of modeling days used in the projections to meet the EPA recommended minimums of 5 or 10 days. Figure 3-1 also includes the number of days daily maximum 8-hour ozone concentrations in the Denver area were greater than a 70 and 75 ppb threshold. Again, the 2004 and 2005 years are relatively clean years with much fewer days greater than the 75 ppb (10 and 28 days) and 70 ppb (29 and 49 days) concentration thresholds than the other years. 2002, 2003 and 2006 have approximately 40 days greater than 75 ppb compared to ~30 days for 2005 and 2007. The 2006 year has the most days greater than 70 ppb (~70 days) with 2002, 2003 and 2007 having ~60 days, 2005 ~50 days and again 2004 being unusually clean with only ~30 days ≥ 70 ppb.

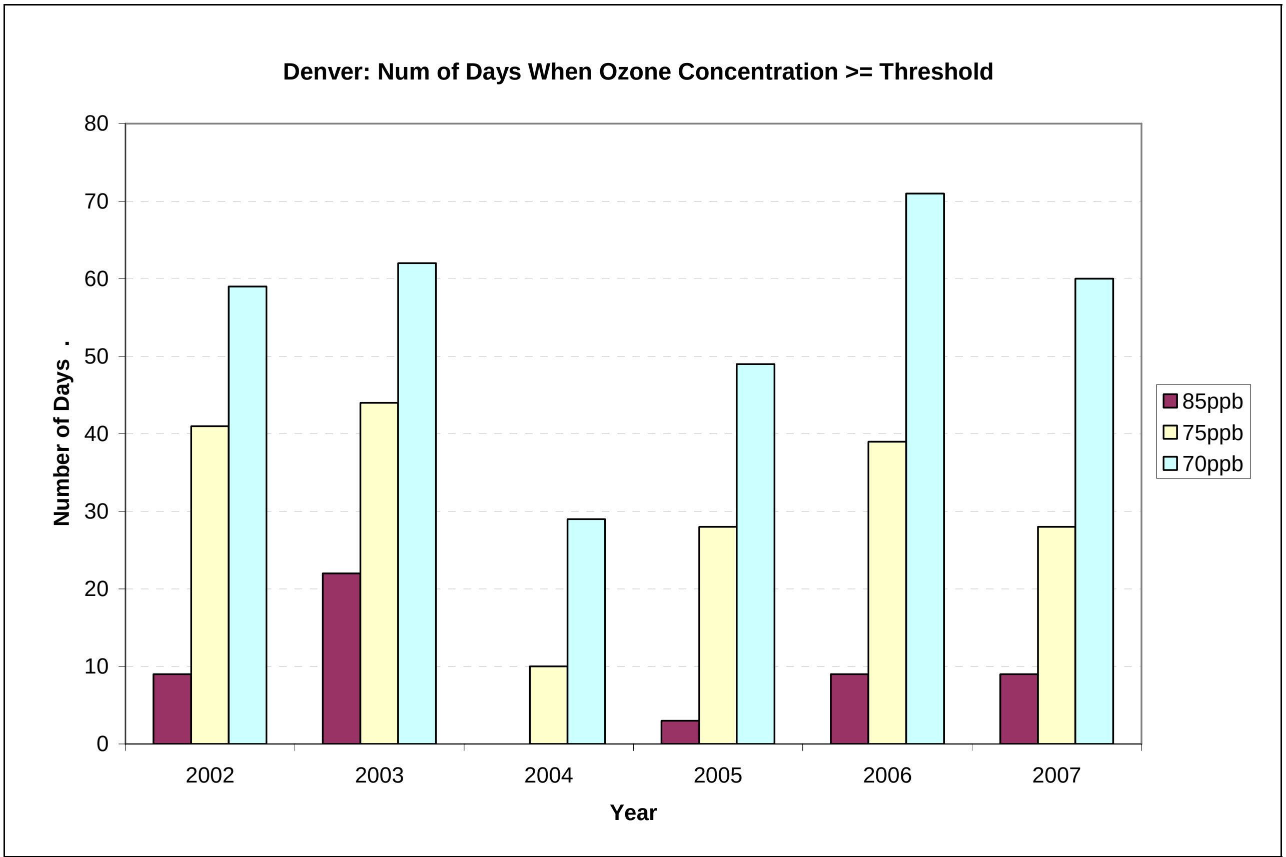


Figure 3-1. Number of days during each of the years from 2002-2007 that the daily maximum 8-hour ozone concentration at any monitor in the Denver area was 85, 75 or 70 ppb or higher.

The RFNO, CHAT, NREL, SBC and FTCW monitoring sites have been identified as key ozone monitors in the Denver area for the 8-hour ozone projections since they all have current (2005-2007) 8-hour ozone DVs in excess of 80 ppb. Figure 3-2 lists similar information as Figure 3-1 only separately for each of these key monitoring sites. As shown previously in Figure 3-1, the years 2004 and 2005 have the lowest number of days with high ozone concentrations at these key monitors (Figure 3-2) and it would be difficult to obtain a sufficient number of high ozone days to meet EPA's minimal criteria for ozone projections. Thus, ozone episodes from the 2004 and 2005 years are not considered for the Denver 8-hour ozone attainment demonstration modeling. The other years appear that they could have sufficient modeled days to meet EPA's minimal day criteria.

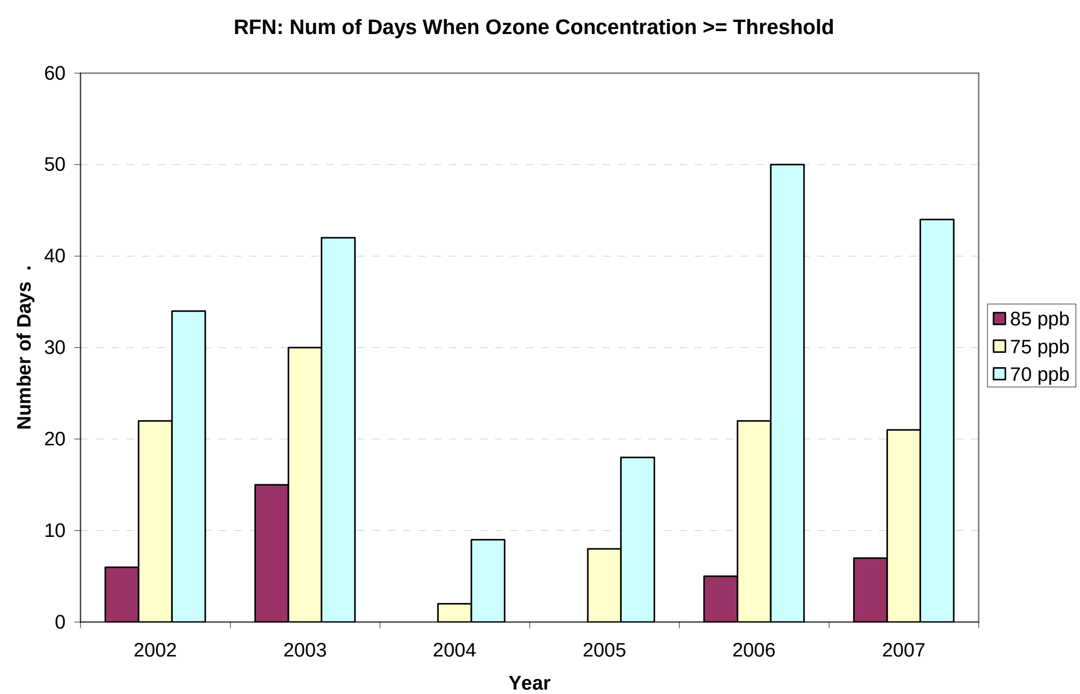


Figure 3-2a. Number of days during each of the years from 2002-2007 that the daily maximum 8-hour ozone concentration at the Rocky Flats North (RFNO) monitor was 85, 75 or 70 ppb or higher

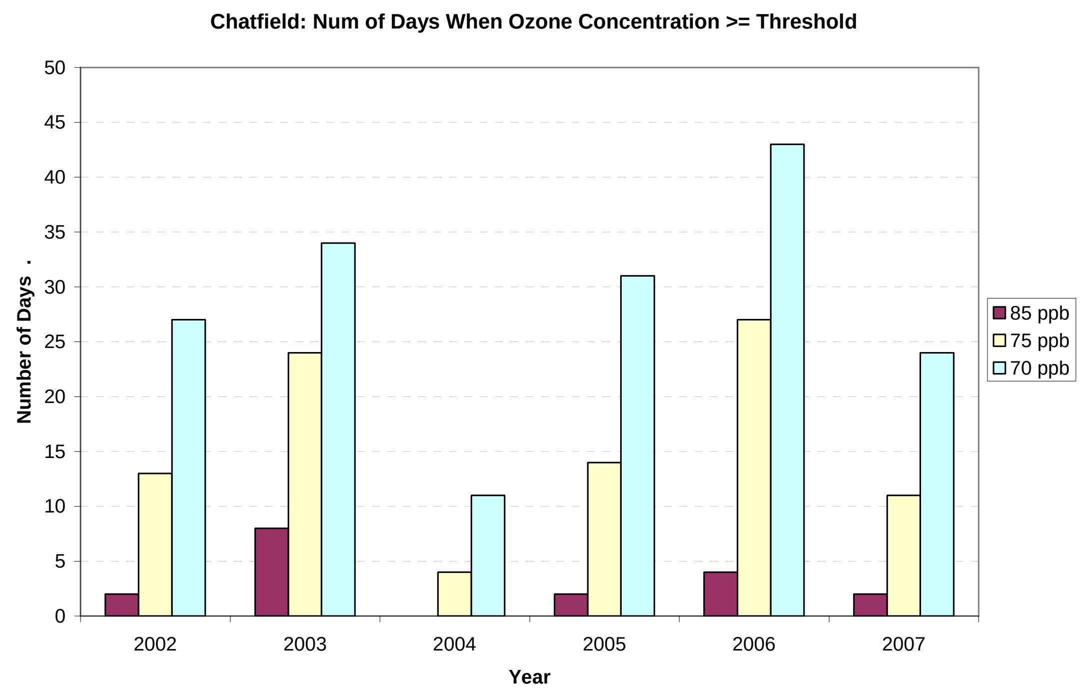


Figure 3-2b. Number of days during each of the years from 2002-2007 that the daily maximum 8-hour ozone concentration at the Chatfield (CHAT) monitor was 85, 75 or 70 ppb or higher

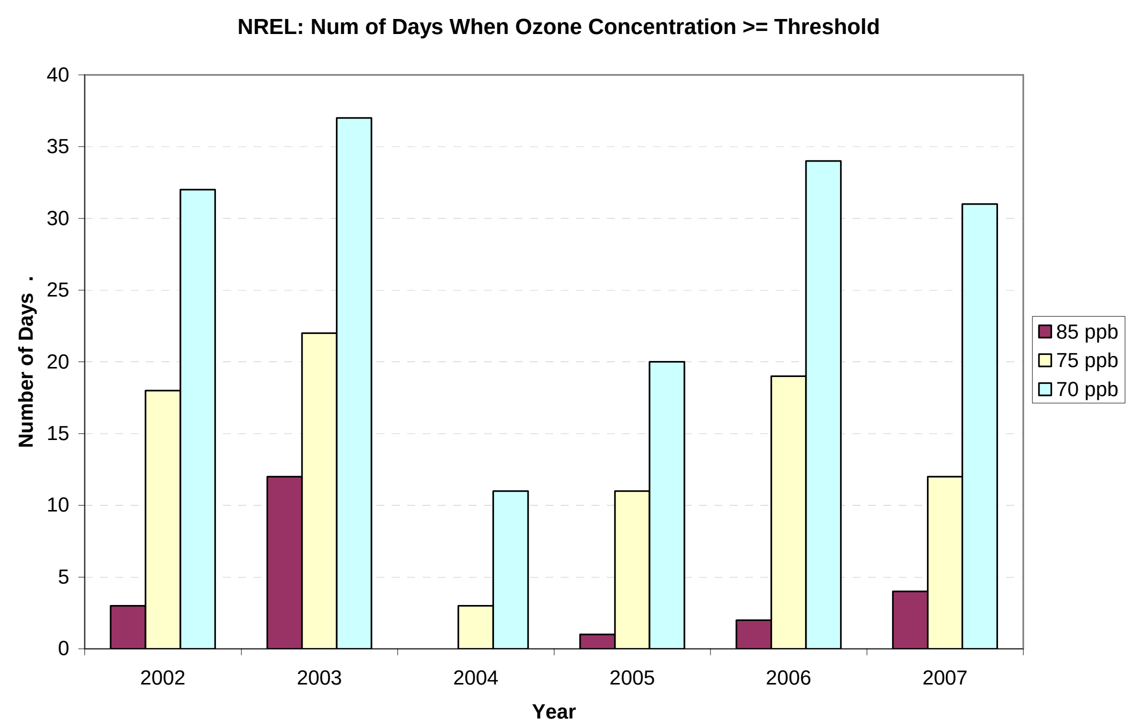


Figure 3-2c. Number of days during each of the years from 2002-2007 that the daily maximum 8-hour ozone concentration at the NREL monitor was 85, 75 or 70 ppb or higher.

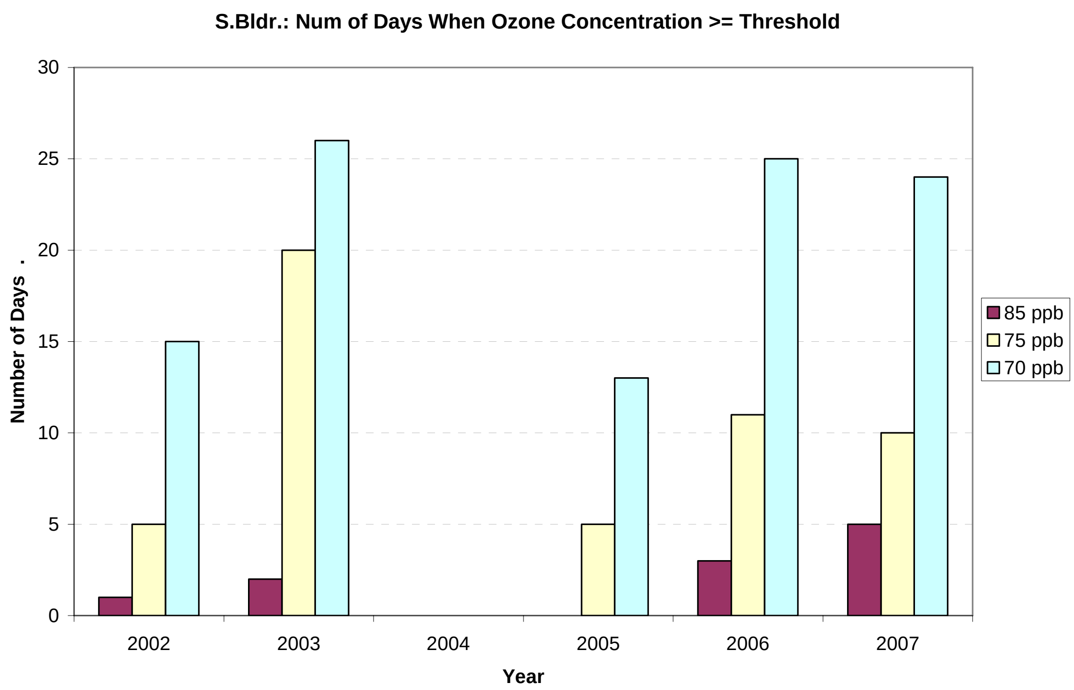


Figure 3-2d. Number of days during each of the years from 2002-2007 that the daily maximum 8-hour ozone concentration at the South Boulder Creek (SBC) monitor was 85, 75 or 70 ppb or higher

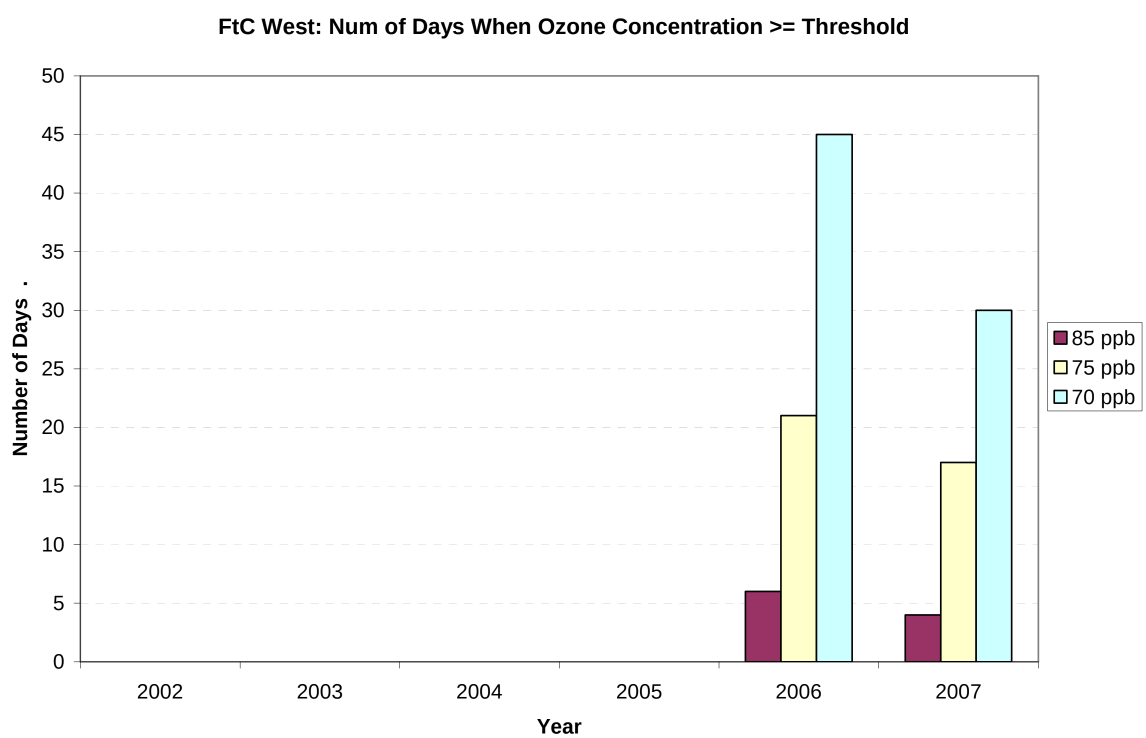


Figure 3-2e. Number of days during each of the years from 2002-2007 that the daily maximum 8-hour ozone concentration at the Fort Collins West (FTCW) monitor was 85, 75 or 70 ppb or higher (data only available for 2006 and 2007).

3.2.4 Daily 8-Hour Ozone Time Series for 2002-2007

Figure 3-3a through 3-3f display time series of daily maximum 8-hour ozone concentrations from the four highest monitors for each day and the years 2002-2007. For each day, the daily maximum 8-hour ozone concentrations across the DMA are ranked and then the four highest values are plotted in these figures. Thus, the lines in these figures do not necessarily represent specific monitoring sites but rather the highest through fourth highest values that occurred on each day. These figures help indicate the magnitude and spatial extent of each high ozone day during the year and whether groups of high ozone days (episodes) occur in bunches so they can be connected by a contiguous modeling period.

For 2002 (Figure 3-3a), most of the high ozone events occurred during June and July with no 8-hour ozone exceedances occurring before June 1 or after July 31 so the June-July 2002 period is a candidate episode for this year. Note that a portion of this period was modeled as part of the Denver EAC SIP modeling and 2002 was also modeled by the WRAP, CENRAP, MRPO, VISTAS and MANE-VU RPOs so satisfies the EPA secondary criteria to select periods already modeled. However, we believe 2002 is too old for the current Denver 8-hour ozone SIP modeling as there have been significance changes in emissions since then, including fleet turnover, implementation of the EAC SIP control measures and expansion of oil and gas production activity in the region.

In 2003 there are a few isolated 8-hour ozone exceedance days in May, but a vast majority of them occur in between July 8 and August 21, 2003 (Figure 3-3b). Although 2003 has the most 8-hour ozone exceedance events of any of the years studied, the severity of the ozone exceedance events during this year is a cause for concern with 8-hour ozone exceedances of 119 and 115 ppb occurring on July 11 and 12, 2003 that were the highest events during the six year period studied (2002-2007). Recall one of the EPA criteria for episode selection is 8-hour ozone concentrations near the current observed maximum DV (85 ppb). Of the 22 exceedance days in 2003 over half have maximum daily maximum 8-hour ozone concentrations in excess of 90 ppb. Like 2002, the 2003 is also likely too old for the current round of Denver 8-hour ozone attainment demonstration modeling.

The daily 8-hour ozone concentration time series for 2004 (Figure 3-3c) and 2005 (Figure 3-3d) confirm the results in Figures 3-1 and 3-2 that these two years are relatively clean ozone years and do not offer good modeling periods for the Denver 8-hour ozone modeling.

The final two years, 2006 (Figure 3-3e) and 2007 (Figure 3-3f), appear to be good candidates for Denver 8-hour ozone attainment demonstration modeling as they both have extended periods of multiple days with elevated ozone concentrations. For 2006 the period of June 1 through July 31 captures all of the 8-hour ozone exceedance days during 2006 as well as a dramatic clean out event of July 5-12, 2006. The modeling of periods of high and low ozone concentrations is desirable as it tests the model’s ability to simulate both high and low ozone conditions; a model that is unable to simulate low ozone conditions may perform well in a base case but be unable to respond to future-year emission controls correctly. The 2007 year also has a good candidate modeling period of June 14 through July 31 with periods of high and low ozone concentrations that can be used to test the model. There is also a high (95 ppb) isolated ozone exceedance event on August 25, 2007. Although the extension of the 2007 episode almost a whole another month to capture a single 8-hour ozone exceedance day does not appear to be good use of computational resources.

Based on the observed ozone concentrations in the Denver area and using EPA's episode selection criteria, either the June-July 2006 or June-July 2007 modeling periods capture sufficient 8-hour ozone episodes and appear to be appropriate modeling periods for the Denver 8-hour ozone SIP attainment demonstration modeling.

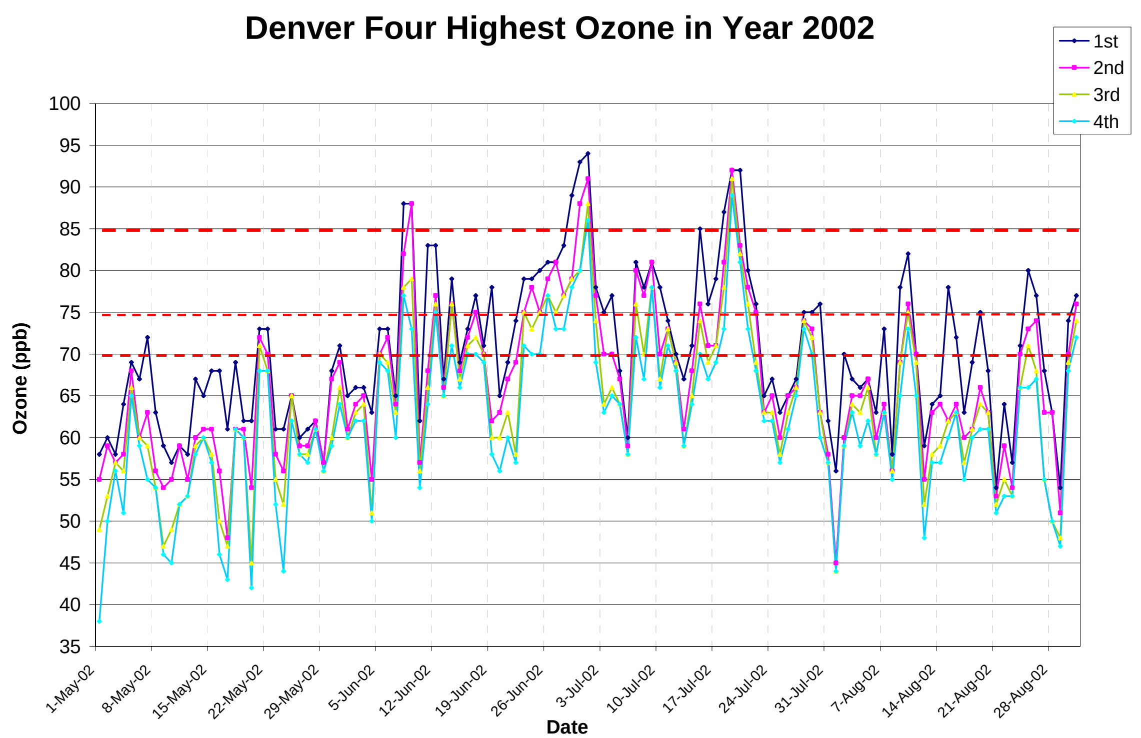


Figure 3-3a. Time series of four highest daily maximum 8-hour ozone concentrations in the Denver area during 2002.

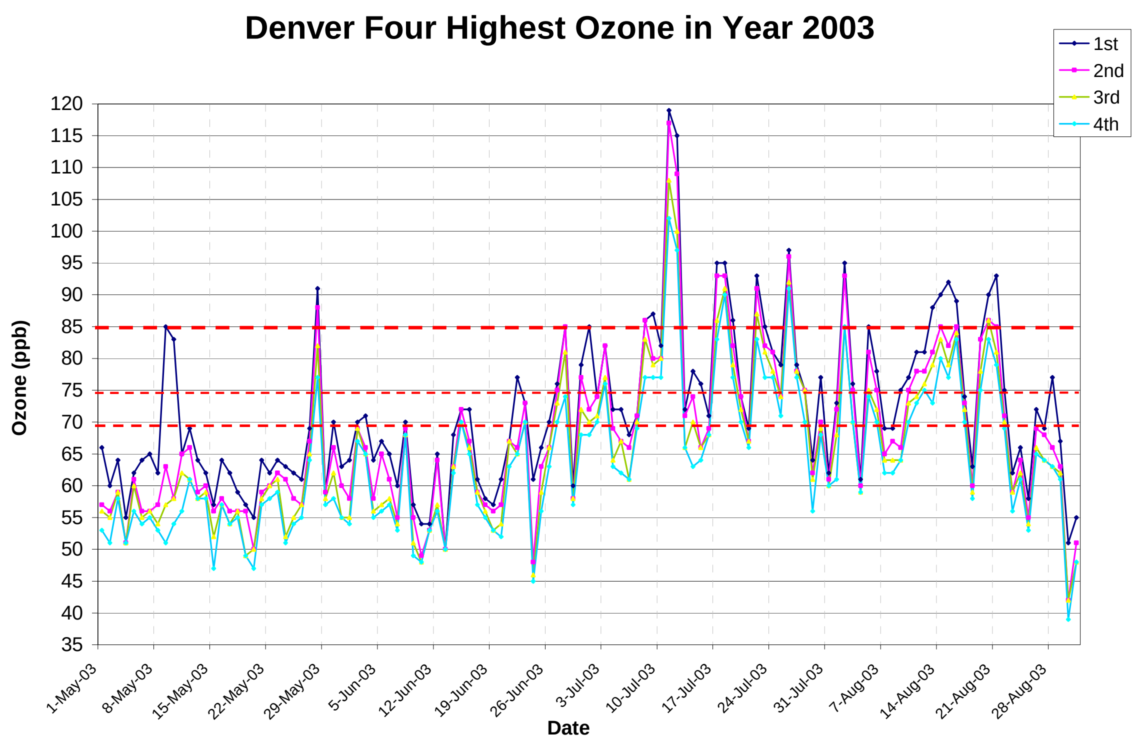


Figure 3-3b. Time series of four highest daily maximum 8-hour ozone concentrations in the Denver area during 2003.

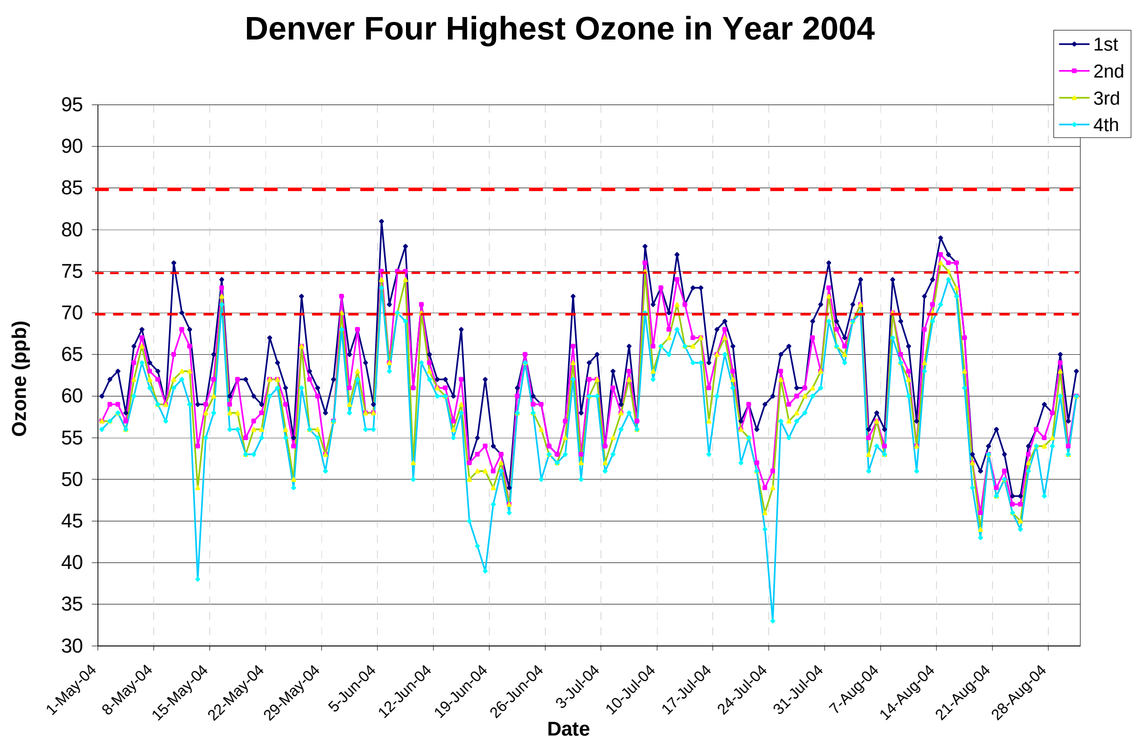


Figure 3-3c. Time series of four highest daily maximum 8-hour ozone concentrations in the Denver area during 2004.

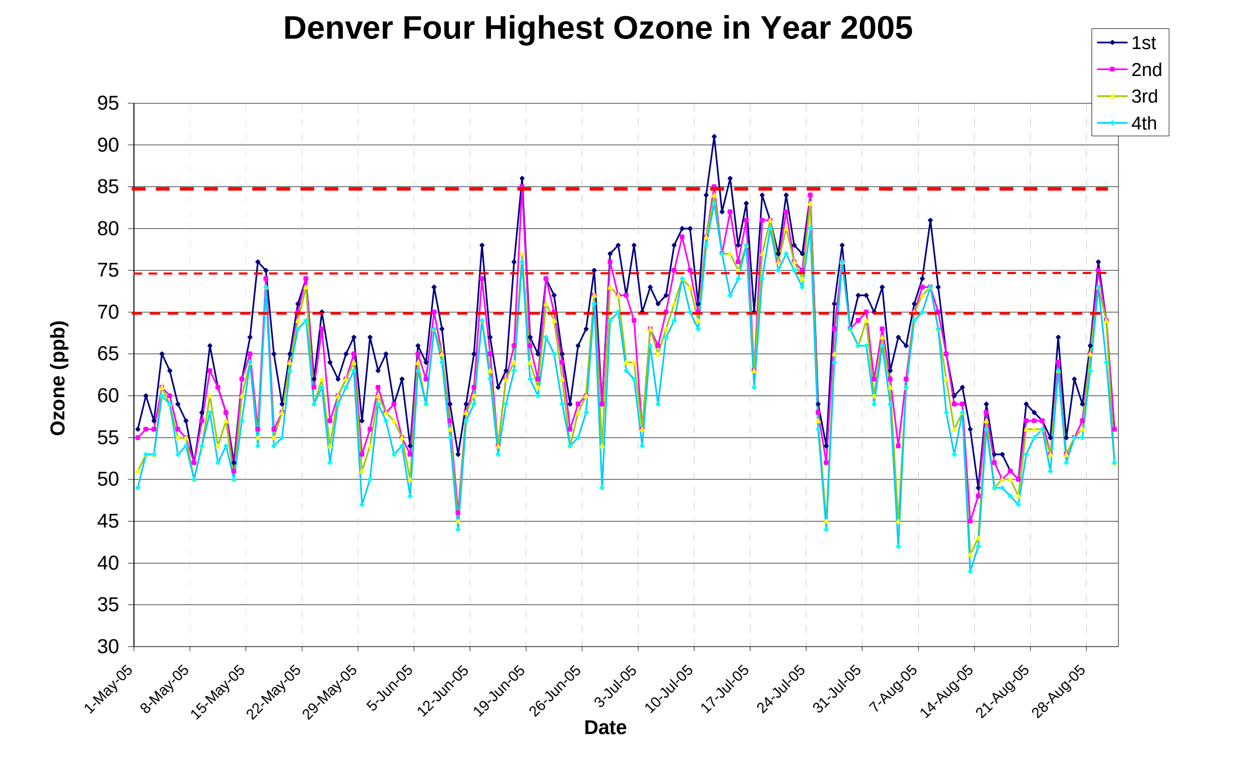


Figure 3-3d. Time series of four highest daily maximum 8-hour ozone concentrations in the Denver area during 2005.

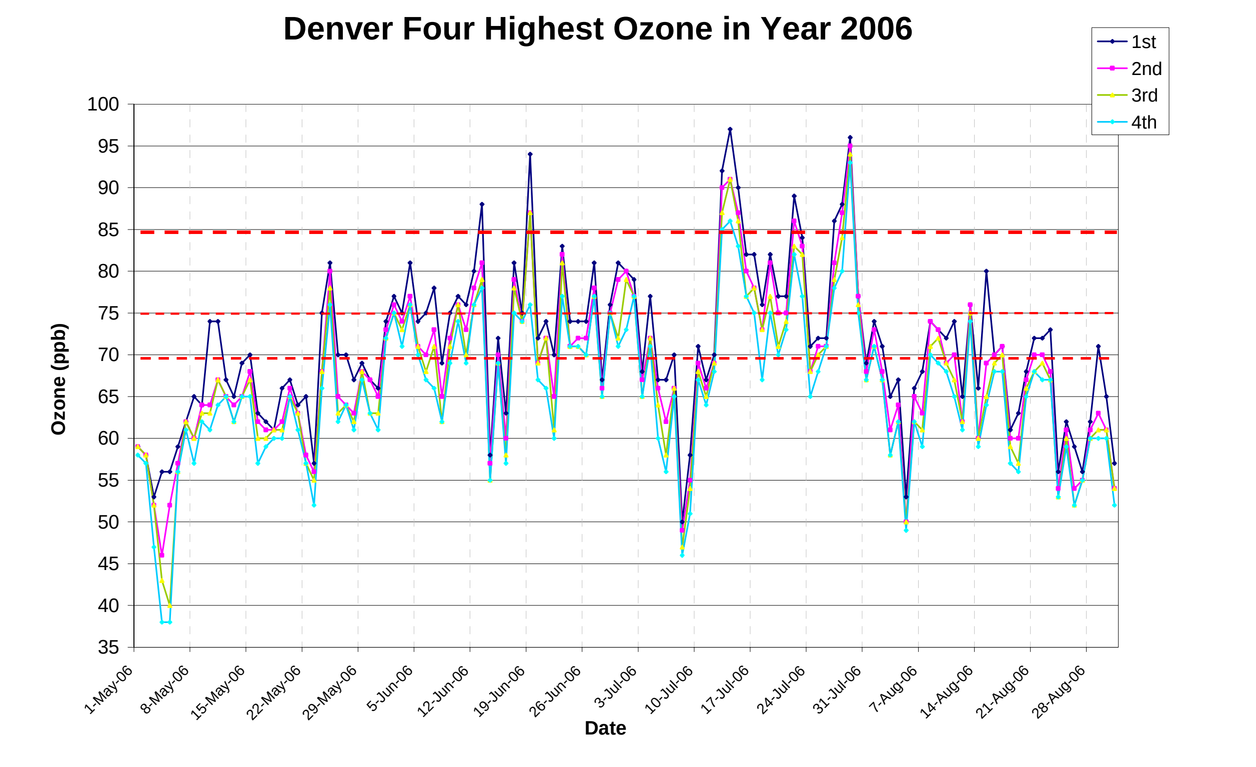


Figure 3-3e. Time series of four highest daily maximum 8-hour ozone concentrations in the Denver area during 2006.

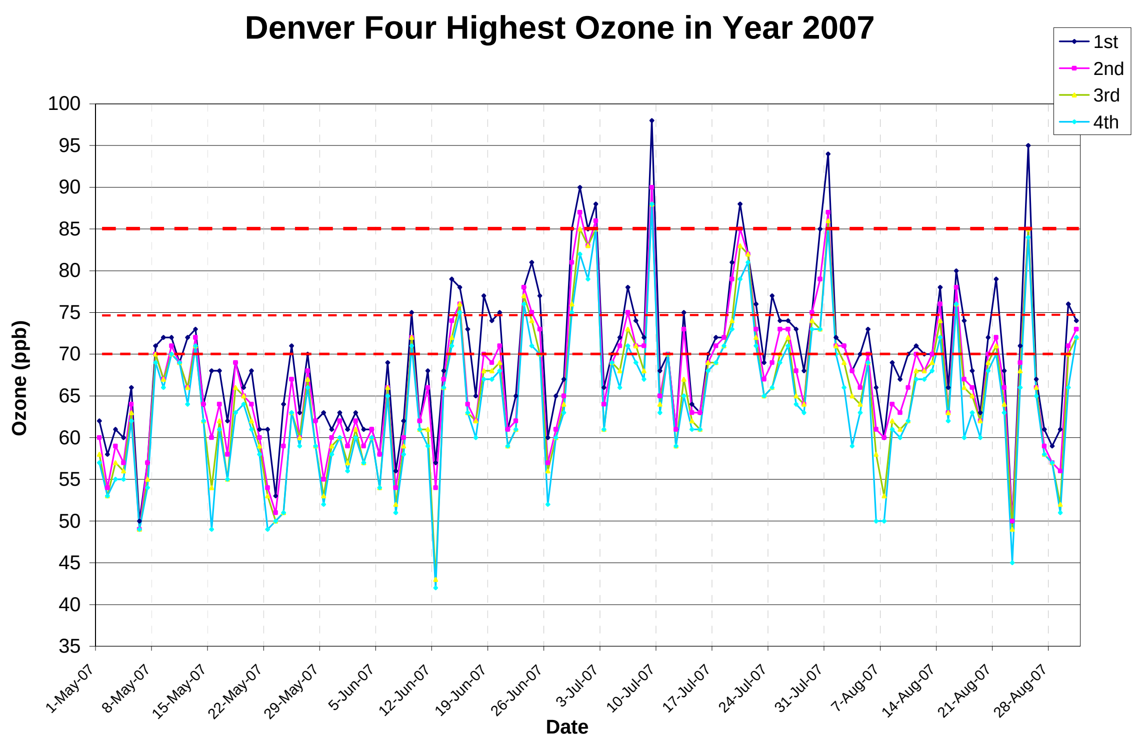


Figure 3-3f. Time series of four highest daily maximum 8-hour ozone concentrations in the Denver area during 2007.

3.3 Final Selection of Denver 8-Hour Ozone Modeling Period

Based on being current and having sufficient number of 8-hour ozone exceedance and high ozone days either the June-July 2006 or June-July 2007 episodes would be appropriate for the Denver 8-hour ozone attainment demonstration modeling. The June-July 2006 modeling period was selected for modeling over the June-July 2007 episode because:

- The June-July 2006 episode has more 8-hour ozone exceedance days (9) than the June-July 2007 episode (8);
- The June-July 2006 episode has substantially more high (> 70 ppb and > 75 ppb) 8-hour ozone days than the June-July 2007 episode (see Figure 3-1);
- There is potentially additional special study data available during the 2006 episode including VOC samples, ozonesondes and ROMANS data; and
- Since it is so recent, not all data will be available for June-July 2007 modeling period in the timeframe required by this study.

This last issue is critical as the 2007 ozone observations will not be fully QA'd for several months and the IMPROVE data for RMNP likely won't be available until some time 2008. Even some of the data needed to run and evaluate the MM5 model may not all be available to properly simulate the 2007 episode.

4.0 MODELING DOMAINS AND DATA AVAILABILITY

This chapter summarizes the model domain definitions for the Denver 8-hour ozone modeling, including the domain coverage, resolution, map projection, and nesting schemes for the high resolution sub-domains. It also discusses the emissions and aerometric data available from various State and federal agencies for use in model input preparation and performance testing.

4.1 Horizontal Modeling Domain

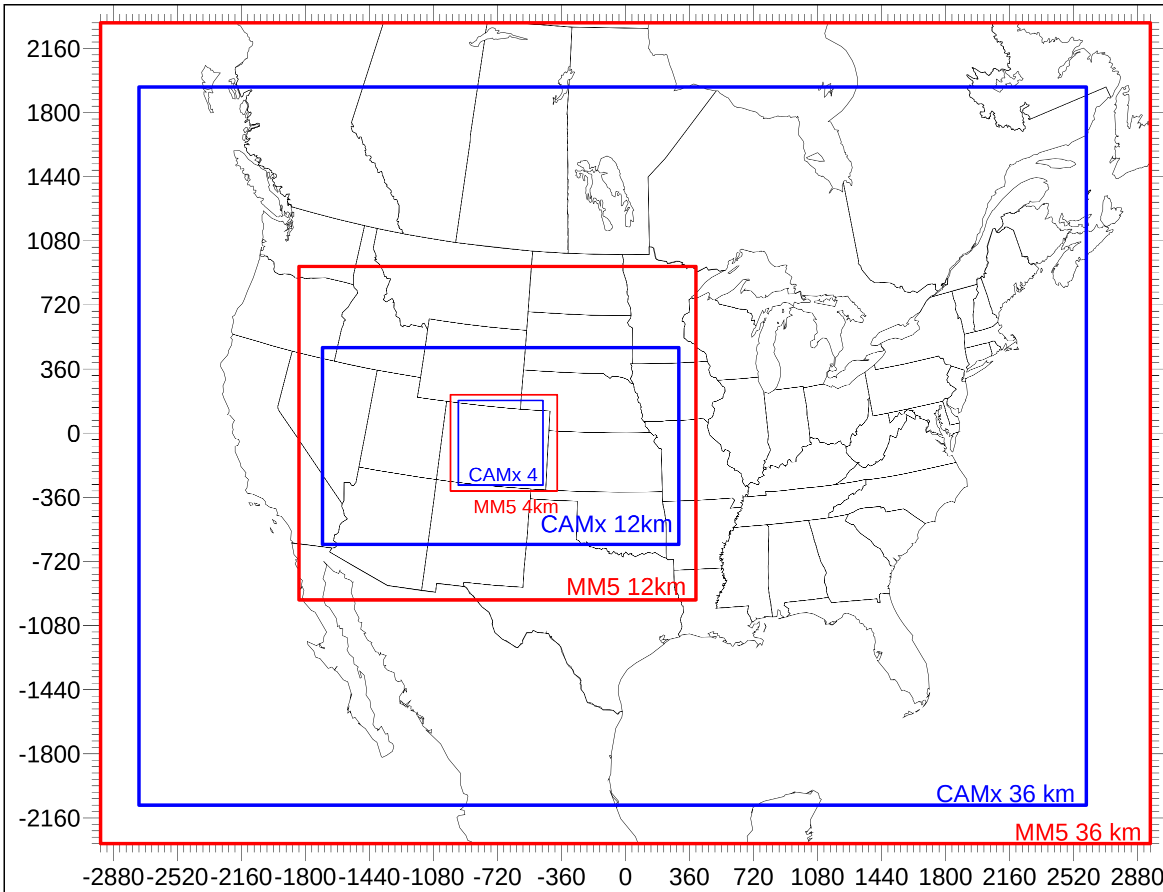
Figure 4-1a displays the 36/12/4 km modeling domains that will be used in the MM5 meteorological and the CAMx/SMOKE air quality/emissions modeling. The 36 km continental United States (U.S.) horizontal domain for CAMx air quality and SMOKE/CONCEPT/MEGAN emissions modeling will be identical to what is used by several Regional Planning Organizations (RPOs) for their regional haze modeling (e.g., WRAP, CENRAP and VISTAS). This 36 km modeling domain covers the continental U.S. as well as large portions of Mexico and Canada.

The MM5 will first be operated on the 36/12 km grid for the May 25 through July 31, 2006 period using two-way grid nesting with feedback (Figure 4-1b). The MM5 results from the 12 km simulation would be used to provide boundary conditions for the 4 km grid that would be operated using one-way grid nesting. MM5 sensitivity simulations will be carried out for the July 20-30, 2006 period and the 4 km grid domain to identify the optimal MM5 configuration for ozone modeling of the Denver area.

The CAMx 36/12/4 km modeling domains are shown in Figure 4-1c. The CAMx 12 km modeling domain includes all of Colorado, Utah, Kansas, Nebraska, and portions of Oklahoma, Texas, New Mexico, Arizona, Nevada, Idaho, Wyoming and South Dakota (Figure 4-1d). The CAMx 4 km modeling domain covers almost all of Colorado (Figure 4-1e).

The CAMx air quality and SMOKE/CONCEPT/MEGAN emissions modeling 36/12/4 km modeling domains are aligned within the MM5 domains. The MM5 modeling domains are offset (larger) from the CAMx/emissions modeling domains by at least 6 grid cells in each direction (Figure 4-1a). These grids are based on a Lambert Conformal Projection (LCP) using the same projection as adopted by the RPOs. The LCP is defined by the projection parameters listed in Table 4-1.

There is a possibility of boundary noise effects resulting from boundary conditions coming into dynamic balance with MM5's algorithms. The larger MM5 domain is designed to sequester such errors from the air quality simulation. The buffer region used here exceeds the EPA suggestion of at least 5 grid cell buffer at each boundary.



Denver Modeling Domain

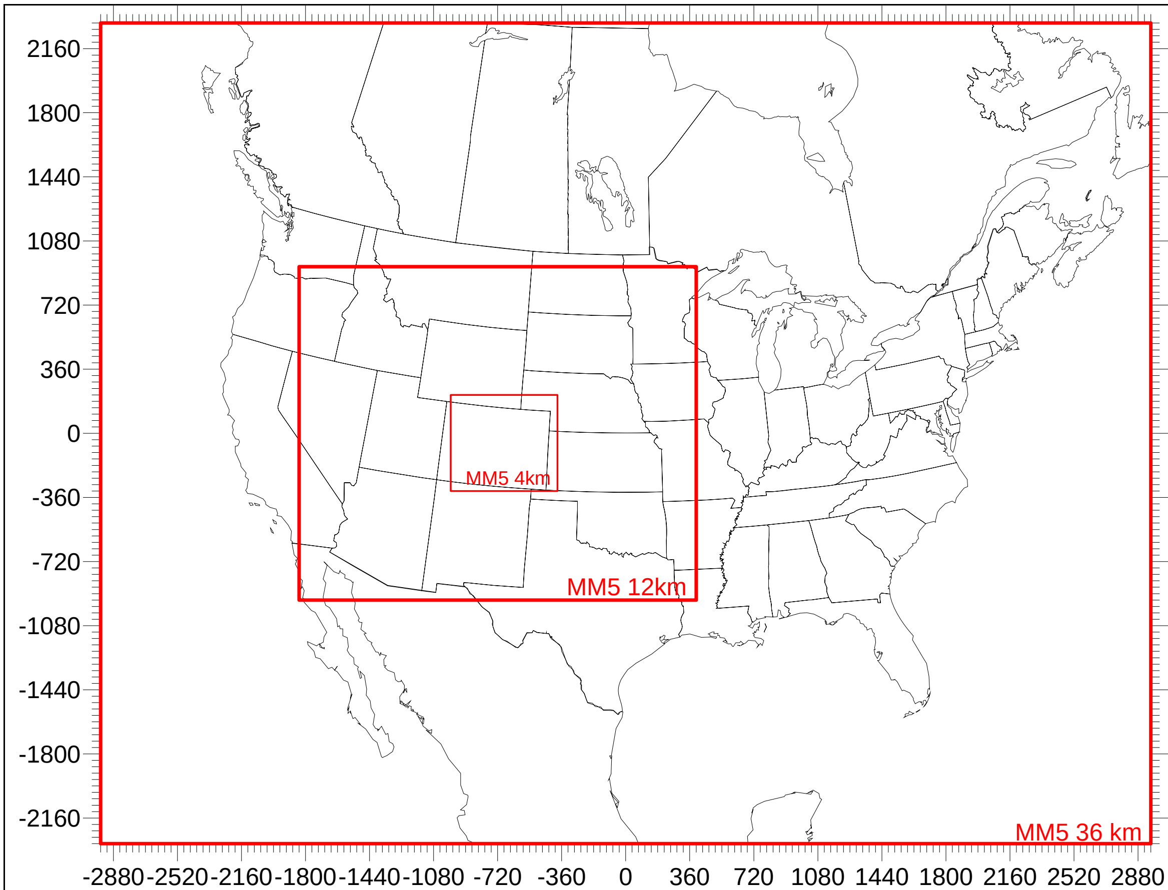
MM5 Domain

36 km: 165 x 129 dot points (-2952, -2304) to (2952, 2304)
12 km: 187 x 157 dot points (-1836, -936) to (396, 936)
04 km: 151 x 136 dot points (-984, -324) to (-384, 216)

CAMx Domain

36 km: 148 x 112 (-2736, -2088) to (2592, 1944)
12 km: 167 x 92 (-1704, -624) to (300, 480)
04 km: 119 x 119 (-940, -292) to (-464, 184)

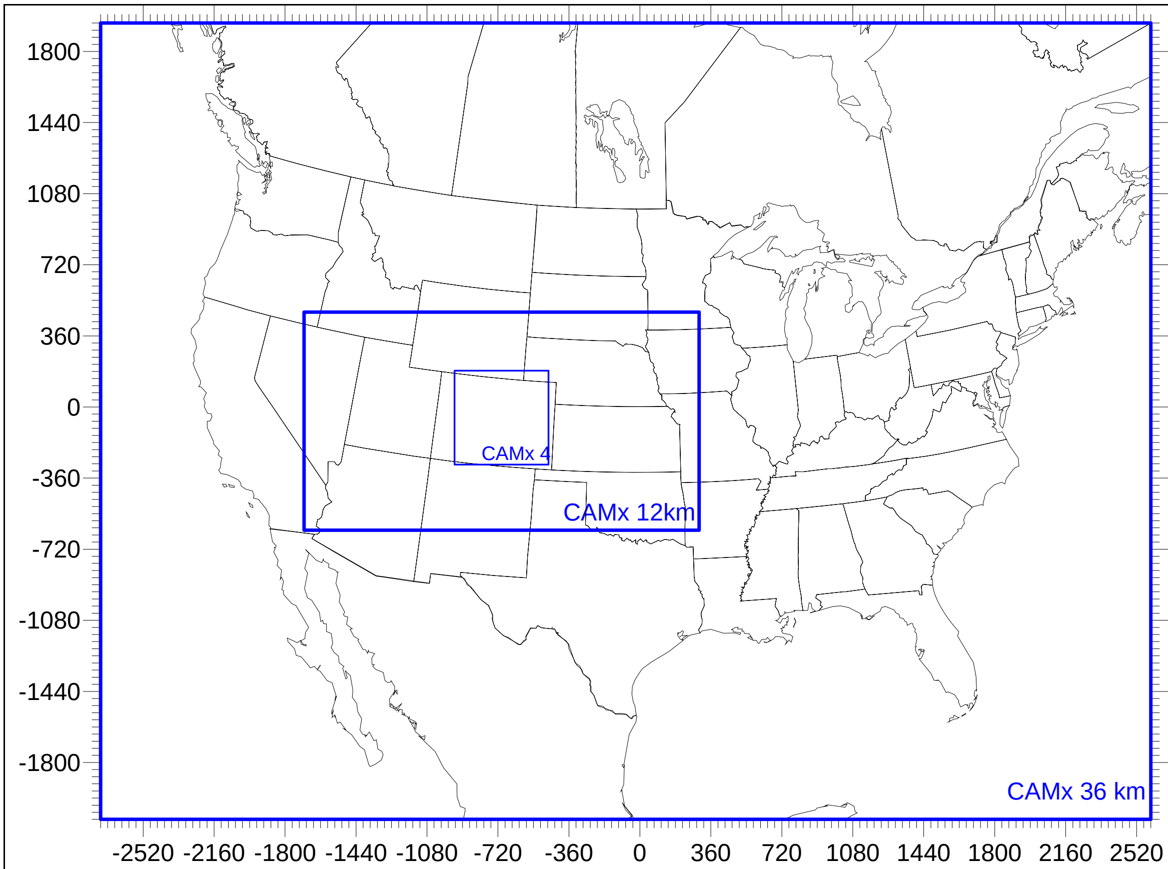
Figure 4-1a. Nested 36/12/4 km modeling domains for the Denver 8-hour ozone modeling study. Blue line domains are for CAMx/SMOKE that are nested in the MM5 red line domains.



Denver MM5 Domain

- 36 km: 165 x 129 dot points (-2952, -2304) to (2952, 2304)
- 12 km: 187 x 157 dot points (-1836, -936) to (396, 936)
- 04 km: 151 x 136 dot points (-984, -324) to (-384, 216)

Figure 4-1b. Nested 36/12/4 km modeling domains for the Denver MM5 meteorological modeling.



Denver CAMx Modeling Domain

□	36 km:	148 x 112	(-2736, -2088) to (2592, 1944)
□	12 km:	167 x 92	(-1704, -624) to (300, 480)
□	04 km:	119 x 119	(-940, -292) to (-464, 184)

Figure 4-1c. Nested 36/12/4 km modeling domains for the Denver CAMx air quality and SMOKE emissions modeling.

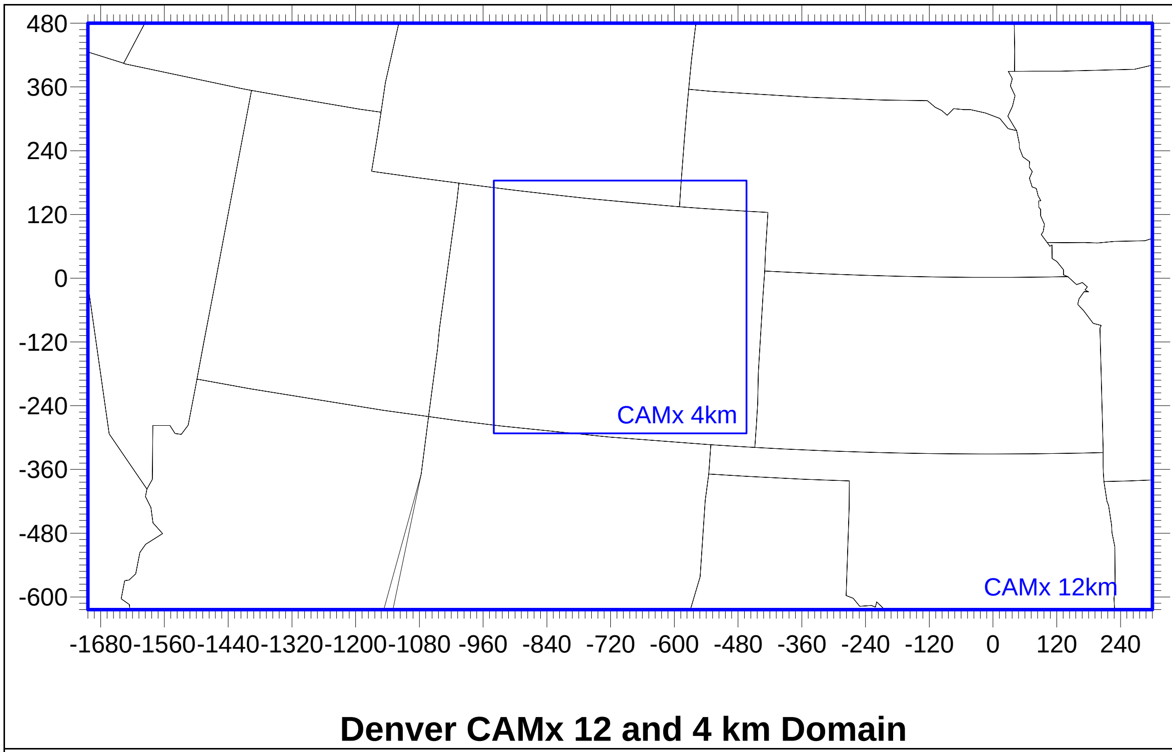
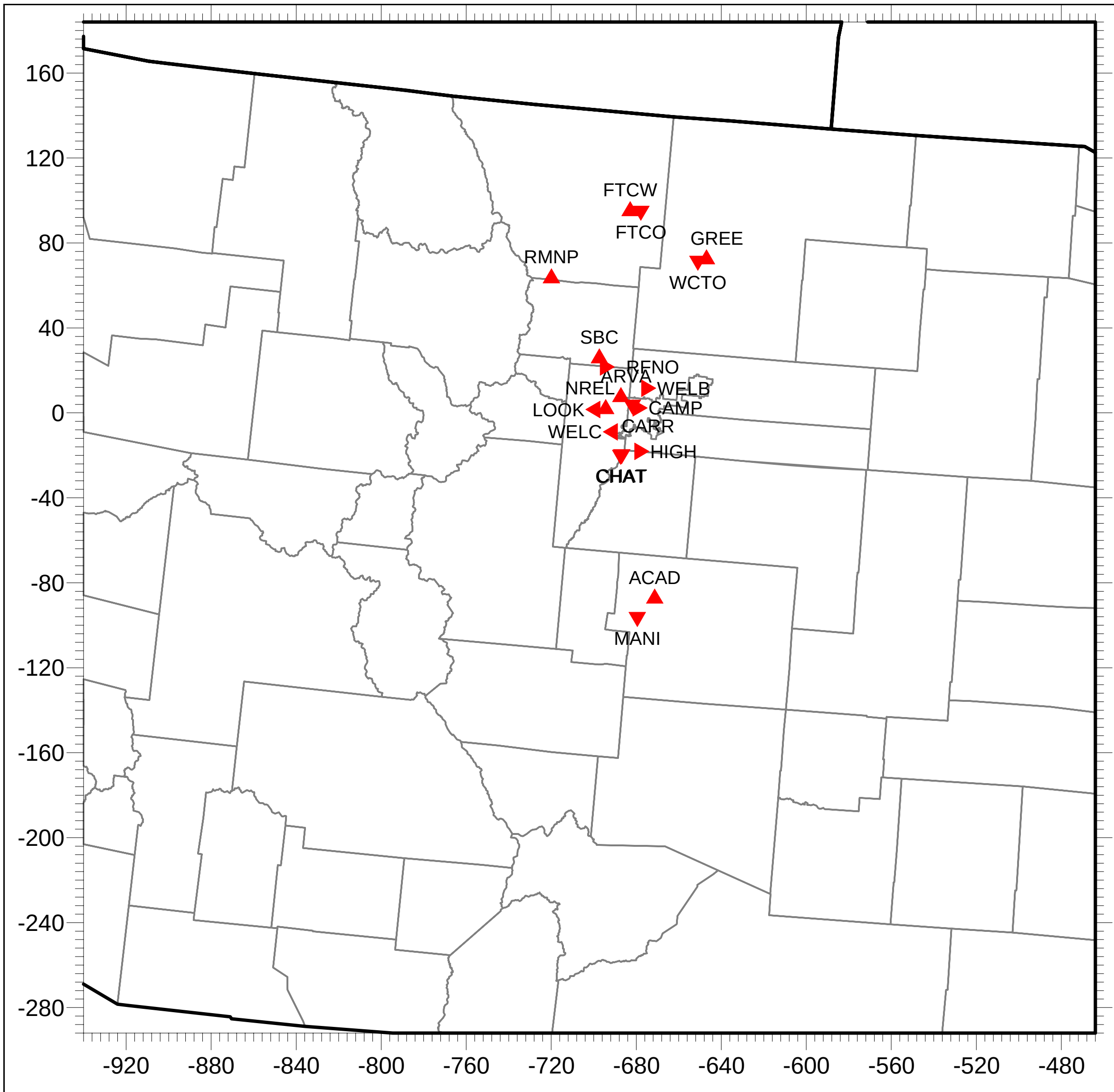


Figure 4-1d. Nested 12/4 km modeling domains for the Denver CAMx air quality and SMOKE emissions modeling.



Denver Ozone Monitoring Sites in the 4 km Domain

Figure 4-1e. Denver 4 km modeling domains for the CAMx air quality and SMOKE emissions modeling and locations of ozone monitoring sites within and near the Denver NAA.

Table 4-1. Lambert Conformal Projection (LCP) definition for the Denver 36/12/4 km modeling grid.

Parameter	Value
Projection	Lambert-Conformal
1st True Latitude	33 degrees N
2nd True Latitude	45 degrees N
Central Longitude	-97 degrees W
Central Latitude	40 degrees N

Table 4-2. Grid definitions for MM5, Emissions and CAMx.

MODEL	COLUMNS DOT(CROSS)	ROWS DOT(CROSS)	XORIGIN (KM)	YORIGIN (KM)
MM5				
36 km grid	165 (164)	129 (128)	-2952.0	-2304.0
12 km grid	187 (186)	157 (156)	-1836.0	-936.0
4 km grid	151 (150)	136 (135)	-984.0	-324.0
Emissions/CAMx				
36 km grid	(148)	(112)	-2736.0	-2088.0
12 km grid	(167)	(92)	-1704.0	-624.0
4 km grid	(119)	(119)	-940.0	-940.0

Table 4-2 lists the number of rows and columns and the definition of the X and Y origin (i.e., the southwest corner) for the 36/12/4 km domains to be used by MM5, CAMx and the SMOKE, CONCEPT and MEGAN emissions models. In Table 4-2 "Dot" refers to the grid mesh defined at the vertices of the grid cells while "Cross" refers to the grid mesh defined by the grid cell centers. Thus, the dimension of the dot mesh is equal to the cross mesh plus one.

4.2 Vertical Modeling Domain

The CAMx vertical structure is primarily defined by the vertical grid used in the MM5 modeling. The MM5 model employs a terrain following coordinate system defined by pressure, using multiple layers that extend from the surface to 100mb (approximately 15 km AGL). A layer averaging scheme is adopted for CAMx simulations to reduce the air quality computational time. The effects of layer averaging were evaluated by WRAP and VISTAS and found to have a relatively minor effect on the model performance metrics when both 34 layer and 19 layer CMAQ model simulations were compared to ambient monitoring data (Morris et al., 2004a). For the Denver ozone modeling, 19 vertical layers will be used. Table 4-3 lists the mapping from the MM5 vertical layer structure to the CAMx vertical layers. This MM5 structure was taken from the WRAP, VISTAS and CENRAP RPO configuration and the same 19 layer CAMx structure is also being used in the RPO modeling.

Table 4-3. Vertical layer definition for MM5 simulations (left most columns), and approach for reducing CAMx layers by collapsing multiple MM5 layers (right columns).

MM5					CAMx			
Layer	Sigma	Pres (mb)	Height (m)	Depth (m)	Layer	Pres (mb)	Height (m)	Depth (m)
34 (top)	0.000	100	18123	2856	19	100	18123	9160
33	0.050	145	15267	2097				
32	0.100	190	13170	1659				
31	0.150	235	11510	1374				
30	0.200	280	10136	1173				
39	0.250	325	8963	1024	18	325	8963	3492
28	0.300	370	7938	909				
27	0.350	415	7030	817				
26	0.400	460	6213	742				
25	0.450	505	5471	680	17	505	5471	1890
24	0.500	550	4791	627				
23	0.550	595	4163	582				
22	0.600	640	3581	543	16	640	3581	1053
21	0.650	685	3038	509				
20	0.700	730	2528	386	15	730	2528	664
19	0.740	766	2142	278				
18	0.770	793	1864	269	14	793	1864	443
17	0.800	820	1596	174				
16	0.820	838	1421	171	13	838	1421	338
15	0.840	856	1251	167				
14	0.860	874	1083	164	12	874	1083	163
13	0.880	892	920	161	11	892	920	161
12	0.900	910	759	79	10	910	759	158
11	0.910	919	680	78				
10	0.920	928	601	78	9	928	601	155
9	0.930	937	524	77				
8	0.940	946	447	76	8	946	447	76
7	0.950	955	371	75	7	955	371	76
6	0.960	964	295	75	6	964	295	75
5	0.970	973	220	74	5	973	220	74
4	0.980	982	146	37	4	982	146	37
3	0.985	987	109	37	3	987	109	37
2	0.990	991	73	36	2	991	73	36
1	0.995	996	36	36	1	996	36	36
0 (ground)	1.000	1000	0	0	0	0	0	0

4.3 Data Availability

The CAMx modeling systems requires emissions, meteorology, surface characteristics, initial and boundary conditions (IC/BC), and ozone column data for defining the inputs.

4.3.1 Emissions Data

The base year emissions inventory for ozone modeling of the 4 km Colorado domain (Figure 4-1e) will be based upon the 2006 emissions for the Denver NAA provided by the CDPHE/APCD and projected 2006 emissions from the latest 2002 emission inventories developed by the RPOs and their states (e.g., Strait, Roe and Vukovich, 2004; MACTEC, 2006; ERG, 2006a,b). For purposes of air quality model performance evaluation, actual day-specific hourly NOx and SO2 emissions for Electrical Generating Units (EGU) and other large stationary sources that have Continuous Emissions Monitoring (CEM) systems will be used. If appropriate and as data are available, day-specific fire activity data will be also be used in the base case simulations used for model evaluation. For strategy and future year emission runs, “typical year” emissions for these categories will be processed for the base and future years.

For outside of Colorado in the 36 km and 12 km domains we will use 2006 VMT data and the SMOKE-MOBILE6 model for on-road mobile sources. 2006 CEM data will be used for all large stationary sources (Primarily EGUs). The MEGAN biogenic emissions model will be used with the 2006 MM5 data to generate biogenic emissions for the 36/12/4 km domains. Existing 2005 project emissions for area, non-road mobile and non-EGU point sources for the portions of the 36/12 km domains outside of Colorado.

Emissions will be converted to Inventory Data Analyzer (IDA) format and the data will be processed for air quality modeling using Version 2.3 of the SMOKE emissions modeling system. The exception to this is for on-road mobile sources in the Denver nonattainment area (NAA) and biogenic emissions. On-road mobile sources in the Denver NAA will be generated using the CONCEPT emissions model and link-based vehicle miles traveled (VMT) data from a travel demand model (TDM) and biogenic emissions will be generated using the MEGAN biogenic emissions model. Included in these runs will be the temporal and speciation profiles and cross-reference data provided with SMOKE, augmented with any recommended and approved emission profile data obtained from EPA, or prepared by the study team prior to initial emissions modeling. Spatial allocation of the emissions will be based on profiles and allocation factors developed for the modeling grid. Additional description of emissions processing is described in Chapter 5.

4.3.2 Air Quality

Data from ambient monitoring networks for gas species are used in the model performance evaluation. Table 4-4 summarizes routine ambient gaseous and PM monitoring networks available in the U.S. Figure 4-2 displays the ozone monitoring sites within and near the Denver area that are also summarized in Table 4-5. Special air quality and air quality related measurements collected in the general Denver area during 2006 include VOC sampling by CDPHE, ozonesondes by NOAA (Cooper et. al., 2007) and data collected as part of the ROMANS study.

Table 4-4. Overview of routine ambient data monitoring networks.

Monitoring Network	Chemical Species Measured	Sampling Period	Data Availability/Source
The Interagency Monitoring of Protected Visual Environments (**IMPROVE**)	Speciated PM_{25} and PM_{10} (see species mappings)	1 in 3 days; 24 hr average	http://vista.cira.colostate.edu/improve/Data/IMPROVE/improve_data.htm
Clean Air Status and Trends Network (**CASTNET**)	Speciated PM_{25}, Ozone (see species mappings)	Approximately 1-week average	http://www.epa.gov/castnet/data.html
National Atmospheric Deposition Program (**NADP**)	Wet deposition (hydrogen (acidity as pH), sulfate, nitrate, ammonium, chloride, and base cations (such as calcium, magnesium, potassium and sodium)), Mercury	1-week average	http://nadp.sws.uiuc.edu/
Air Quality System (**AQS**) or Aerometric Information Retrieval System (**AIRS**)	CO, NO2, O3, SO2, PM_{25}, PM_{10}, Pb	Typically hourly average	http://www.epa.gov/air/data/
Speciation Trends Network (**STN**)	Speciated PM	24-hour average	http://www.epa.gov/ttn/amtic/amticpm.html
Southeastern Aerosol Research and Characterization (**SEARCH**) (Southeastern US only)	24-hr PM25 (FRM Mass, OC, BC, SO4, NO3, NH4, Elem.); 24-hr PM coarse (SO4, NO3, NH4, elements); Hourly $PM_{2.5}$ (Mass, SO4, NO3, NH4, EC, TC); Hourly gases (O3, NO, NO2, NOy, HNO3, SO2, CO)	Hourly or 24-hour average, depending on parameter.	Electric Power Research Institute (EPRI), Southern Company, and other companies. http://www.atmospheric-research.com
EPA Particulate Matter Supersites(Includes St. Louis, Pittsburgh, Baltimore, Atlanta and New York in the Denver modeling domain)	Speciated PM25		http://www.epa.gov/ttn/amtic/supersites.html
Photochemical Assessment Monitoring Stations (**PAMS**)	Varies for each of 4 station types.		http://www.epa.gov/ttn/amtic/pamsmain.html
National Park Service Gaseous Pollutant Monitoring Network	Acid deposition (Dry; SO4, NO3, HNO3, NH4, SO2), O3, meteorological data	Hourly	http://www2.nature.nps.gov/ard/gas/netdata1.htm

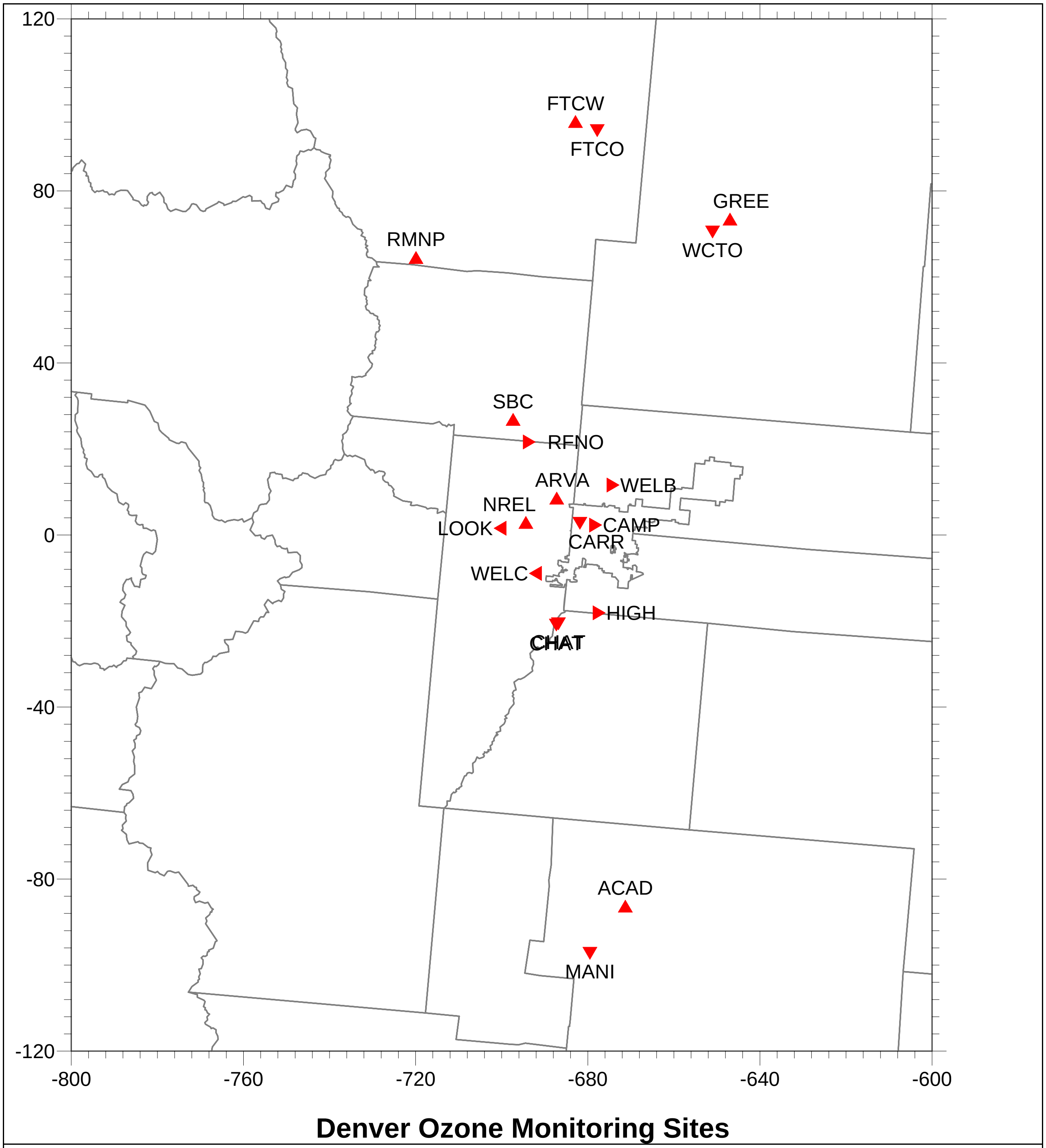


Figure 4-2. Locations of ozone monitoring sites within and near the Denver area.

Table 4-5. Ozone monitoring sites within and near the Denver area operating during 2002-2007.

ID Number	Site Name	Site ID	2002	2003	2004	2005	2006	2007	Lat	Long
080013001	Welby	WELB	x	x	x	x	x	x	39.838	-104.950
080050002	Highland	HIGH	x	x	x	x	x	x	39.568	-104.957
080130011	S. Boulder Creek	SBC	x	x	x	x	x	x	39.957	-105.238
080310002	CAMP	CAMP				x	x	x	39.751	-104.988
080310014	Carriage	CARR	x	x	x	x	x	x	39.752	-105.031
080350002	Chatfield #1	CHAT	x	x	x				39.538	-105.065
080350004	Chatfield #2	CHAT			x	x	x	x	39.534	-105.070
080410013	USAF Academy	ACAD	x	x	x	x	x	x	38.958	-104.817
080410016	Manitou Springs	MANI			x	x	x	x	38.853	-104.901
080590002	Arvada	ARVA	x	x	x	x	x	x	39.800	-105.100
080590005	Welch	WELC	x	x	x	x	x	x	39.639	-105.139
080590006	RFN	RFNO	x	x	x	x	x	x	39.913	-105.189
080590011	NREL	NREL	x	x	x	x	x	x	39.744	-105.178
080590012	Lookout Mountain	LOOK			x				39.727	-105.247
080690007	RMNP	RMNP	x	x	x	x	x	x	40.277	-105.545
080690011	FtC West	FTCW					x	x	40.593	-105.141
080691004	Ft. Collins	FTCO	x	x	x	x	x	x	40.577	-105.079
081230007	Greeley	GREE	x						40.416	-104.692
081230009	Weld Co. Tower	WCTO	x	x	x	x	x	x	40.386	-104.737

4.3.3 Ozone Column Data

Additional data used in the air quality modeling include ozone column data from the Total Ozone Mapping Spectrometer (TOMS) satellite platform. TOMS data are available for 24-hour average time periods, and are obtained from http://toms.gsfc.nasa.gov/eptoms/ep.html. The TOMS data are used in the CAMx (TUV) radiation models to calculate photolysis rates. Frequently TOMS ozone column data are missing for extended periods so data needs to be filled. The CAMx TUV processor allows for the use of episode average data. If there are large periods of missing TOMS data during a Denver June-July 2006 modeling period, then we may use monthly or episode average TOMS data to work around the missing data.

4.3.4 Meteorological Data

Meteorological data are being generated using the MM5 prognostic meteorological model. MM5 runs will be performed on the 36/12/4 km domains and the June-July 2006 period. Initialization days prior to the Denver modeling period will be run on the 36-km grid for 5 days prior to the start of the Denver modeling period. The MM5 model will be started approximately 12 hours prior to the first hour that the data will be used by CAMx.

4.3.5 Initial and Boundary Conditions Data

For the Denver ozone simulations we will use a minimum 5-day initialization period on the 36-km grid to eliminate the contribution of initial concentrations. Clean or other appropriate initial conditions (ICs) will be used at the start of the 5-day initialization period. We will determine an appropriate source for the CAMx boundary conditions (BCs) along the lateral boundaries of the 36 km continental U.S. modeling domain. BCs for the 12 km CAMx domain will be based on the 36 km domain CAMx simulations results using one-way nesting. For most simulations the CAMx 12/4 km grid configuration will be run using two-way interactive grid nesting. However, some sensitivity simulations may also be run using just the 4 km grid with BCs based on the 12 km CAMx simulation.

5.0 MODEL INPUT PREPARATION PROCEDURES

This section describes the procedures to be used in developing the meteorological, emissions, and air quality inputs to the CAMx model for the Denver 8-hour ozone modeling on the 36/12/4 km grids. The development of the CAMx meteorological and emissions inputs are discussed together with the science options recommended for MM5 and CAMx models. The procedures for developing the initial and boundary conditions and photolysis rates inputs are also discussed along with the model application procedures.

The procedures set forth here are consistent with EPA guidance (e.g., EPA, 1991; 1999; 2005a; 2007), other recent 8-hour ozone modeling studies conducted for various State and local agencies using these or other state-of-science modeling tools (see, for example, Morris et al., 2004a,b, 2005a,b; Tesche et al., 2005a,b), as well as the methods used by EPA in support of the recent Clean Air Interstate Rule (EPA, 2005b) and the Clean Air Mercury Rule (EPA, 2005c).

5.1 Meteorological Inputs

5.1.1 MM5 Model Science Configuration

The MM5 model configuration will be based on recent modeling research and sensitivity testing carried out with the MM5 in the western U.S. for WRAP (Kemball-Cook et al., 2004), the Denver EAC (McNally, Tesche and Morris, 2003) and the ROMANS study (Gebhart et al., 2007), work at the Iowa Department of Natural Resources (Johnson, 2004; 2007), Olerud and co-workers with the VISTAS program (Olerud and Sims, 2004a,b), EPA CAIR modeling (McNally, 2003) and MM5 modeling to support 8-hour ozone EAC SIP development in Texas, Oklahoma, and New Mexico (Morris et al., 2005d).

5.1.2 MM5 Input Data Preparation Procedures

A brief summary of the MM5 input data preparation procedures we will use are listed below and provided in Table 5-1.

Model Selection: The current version of the non-hydrostatic MM5 (version 3.7) will be used. The MM5 TERRAIN, PREGRID/REGRID, RAWINS/little_r, and INTERPF processors will be used to develop model inputs. We considered using the new Weather Research Forecast (WRF) model that is a replacement to MM5. Although it has been extensively applied for forecast applications, its applications for modeling historical air pollution episodes have been limited.

Horizontal Domain Definition: The computational domain on which MM5 will be applied will be sufficiently sized to accommodate the air quality and emissions modeling grids as defined in Figure 4-1 and Tables 4-1 and 4-2 and earlier. The MM5 36/12/4 km domains are defined with at least a 6 grid cell buffer in all directions from the air quality modeling domains.

Table 5-1. MM5 (Version 3.7:4) model configuration.

Science Options	Configuration	Details
Model Code	MM5 version 3.7.4 (MPP) -- 16 Oct. '06	Dudhia (1993), Grell et al., (1994)
Horizontal Grid Mesh	36/12/4 km	
36 km grid	145 x 101 cells	Cross Points (add one for dot points)
12 km grid	163 x 130 cells	
4 km grid	227 x 88 cells	
Vertical Grid Mesh	34 Layers; Surface layer ~ 35 m deep	Vertically varying; sigma pressure coordinate
Domain Depth	Surface to ~15 km AGL	Top defined by 100 mb
Grid Interaction	Feedback	Two-way nesting with feedback
Initialization	EDAS	Eta Data Assimilation System
Boundary Conditions	EDAS	40 km resolution
Microphysics	Mixed Phase Moisture Scheme	Reisner II in 36/12/4 km grids
Cumulus Scheme	Kain-Fritsch 2 subgrid scale cumulus	36/12 km grids only
Planetary Boundary Layer	ACM	Asymmetric Convective Mixing with PX LSM
Radiation	RRTM	Rapid Radiative Transfer Model
Vegetation & Land Use	USGS	24 Category Scheme
36 km grid	10 min (~18 km) global data	Geophysical Data Center
12 km grid	5 min (~9 km) global data	Geophysical Data Center
4 km grid	High-Resolution (30 sec)	NCAR
Land Surface Model	Pleim-Xiu LSM (ISOIL = 3)	Soil moisture from EDAS fields, not PX module
Topographic Input		
36/12/4 km grid	Updated NCAR/PSU data bases	Supplied with MM5
Shallow Convection	None	
Sea Surface Temperature	EDAS skin temperature	Spatially varying
4D Data Assimilation		
36 km grid	Analysis nudging wind, temp and moisture above PBL, only wind below PBL	Wind, temp coeff = 2.5x10-4; mixing ratio coeff = 1x10-5
12 km grid	Analysis nudging wind, temp and moisture above PBL, only wind below PBL	Wind, temp coeff = 2.5x10-4; mixing ratio coeff = 1x10-5
4 km grid	Analysis nudging wind, temp and moisture above PBL, only wind below PBL. Surface wind observation nudging.	Wind, temp coeff = 2.5x10-4; mixing ratio coeff = 1x10-5
Spin-up	Spin-up time typically ~12 hrs	Spin-up prior to ozone episode simulation

Vertical Domain Definition: The MM5 modeling will employ 34 vertical layers with an approximately 36 meter deep surface layer, based upon the configuration used in the CENRAP modeling. The MM5 vertical domain is presented in both sigma and height coordinates in Table 4-3.

Topographic Inputs: Topographic information for the MM5 will be developed using the NCAR and the U.S. Geological Survey (USGS) terrain databases. The 36-km grid will be based the 10 min (~18 km) Geophysical Data Center global data. The 12-km grid will be developed from the 5 min (~9 km) Geophysical Data Center global data, whereas the 4-km terrain heights will be based on 30 second data (~1 km resolution). Terrain data will be interpolated to the model grid using the TERRAIN pre-processor.

Vegetation Type and Land Use Inputs: Vegetation type and land use information will be developed for the 36/12/4 km grids using the most recently released NCAR/PSU databases provided with the MM5 distribution. Standard MM5 surface characteristics corresponding to each land use category will be employed.

Atmospheric Data Inputs: Initialization, boundary conditions and FDDA nudging fields will be based on the 40 km Eta Data Assimilation System (EDAS) fields.

Water Temperature Inputs: The EDAS "skin temperature" field will be used for water temperature inputs.

FDDA Data Assimilation: Standard FDDA data assimilation techniques will be used in this study (see, for example, Johnson 2004, 2007; Nielson-Gammon et al., 2005; Olerud and Simms, 2004a,b;and Gao et al., 2000; Kemball-Cook et al., 2005). The MM5 simulations will use the three-dimensional analysis-nudging technique where the predictions are nudged toward a field prepared by regridding the EDAS. For these simulations a nudging coefficient of $2.5x10^{-4}$ will be used for winds and temperature and $1x10^{-5}$ for mixing ratio on the 36/12/4 km grids. Thermodynamic variables will *not* be nudged within the boundary layer (i.e., only winds will be nudged within the PBL). In the 4-km grid, surface observation nudging will be performed for winds only.

Nesting Configuration: MM5 will first be run for the May 25 – July 31, 2006 period on the 36/12 km grids using two-way nesting with feedback. The 12 km MM5 output will be processed to generate boundary conditions (BCs) for the 4 km Colorado grid. MM5 will then be run for the June-July 2006 period on the 4 km grid using one-way nesting.

Run Segments: The MM5 simulation will be performed using overlapping 5½ day run segments initialized off of the Eta analysis fields and observed soil moisture. The first half day of the 5½ day run segments would not be used in the CAMx modeling.

Physics Options: The initial MM5 model physics to be used in the MM5 simulations will be as follows:

- Kain Fritsch II cumulus parameterization;
- ACM PBL that is compatible with the PX LSM;
- Plein-Xiu (P-X) Land Surface Model;

- Reisner II Mixed Ice Moisture Scheme; and
- RRTM Atmospheric Radiation Scheme.

Sensitivity Tests: MM5 sensitivity tests will be conducted for the July 20-30, 2006 period and the 4 km grid. The following variables will be considered in the sensitivity modeling:

- Planetary Boundary Layer (PBL) scheme (e.g., ACM, MRF, Blackadar, Eta).
- Land Surface Module (LSM) (e.g., PX, NOAH).
- Cumulus Parameterization (e.g., KF2, KF1, none).
- Moisture (e.g., Reisner 1 and 2).
- Data Assimilation (analysis only, surface wind observations).
  Other

Final MM5 Simulation: The MM5 configuration that performs best will be rerun on the 4 km grid for the entire June-July 2006 modeling period. Performance would be based on both the MM5 meteorological and CAMx air quality model performance for the July 20-30, 2006 period.

5.1.3 MM5CAMx Reformatting Methodology

The MM5CAMx processor maps MM5 meteorological fields to the format required by CAMx. It also calculates turbulent vertical exchange coefficients (Kz) that define the rate and depth of vertical mixing in CAMx. Steps in the MM5CAMx processing include:

- Reading in meteorological model output files;
- Extracting meteorological data for CAMx domain;
- Collapsing meteorological data if coarser vertical resolution data is requested in CAMx than used in MM5;
- Computing vertical diffusivities (Kz) using three options available to the user;

When feasible it is desirable to use the same layer structure in the air quality model as in the MM5 to prevent errors associated with averaging layer data, and to maintain consistency between data produced by the meteorological model and those used by the chemistry-transport model. However, vertical layer collapsing is typically used to reduce computational costs associated with using large number of vertical layers. We propose to reduce the number of vertical layers in the CAMx modeling from 34 to 19. Further details on the CAMx modeling domain definitions were provided in Chapter 4 (Table 4-3).

Two sets of vertical turbulent diffusivity options will be invoked in MM5CAMx from the MM5 ACM/P-X runs: (a) the O'Brien scheme (OB70), and (b) the CMAQ-like scheme. A third option (the TKE method) could also be invoked if the MM5 Eta PBL is used in a sensitivity test. MM5CAMx will be operated initially with a 0.1 m^2/s minimum K_V (Kz_min) value.

5.1.4 Treatment of Minimum K_V

The minimum K_V value (Kz_min) is an area of ongoing investigation by the CAMx model developers and the scientific user community (e.g., CMAQ developers). EPA initially recommended a 1.0 m^2/s Kz_min for CMAQ modeling. However in their ozone forecasting, EPA uses Kz_min values that vary from 0.1 to 2.0 m^2/s depending on the amount of urban land use present. To maximize flexibility we will process the MM5 data using MM5CAMx using a 0.1 m^2/s Kz_min and then test other Kz_min values (e.g., 1.0 m^2/s). The CAMx modeling system contains a utility that produces enhanced minimum Kz (Kz_min) values near the surface to account for increased mixing due to roughness and the urban heat island. The selection of the Kz profiles (O'Brien or CMAQ) and Kz_min approach will be based on the latest thinking, CAMx sensitivity tests and model performance and will be justified in the interim and final documentation on the modeling.

5.2 Emission Inputs

5.2.1 Available Emissions Inventory Datasets

Two 2006 baseline emissions inventories will be developed corresponding to "Actual" and "Typical" emissions. The differences in the Actual and Typical 2006 base case emissions will be in the emissions from large stationary sources with Continuous Emissions Monitoring (CEM) systems and, possibly, wildfire emissions. In the 2006 Actual base case emissions scenario the actual day-specific hourly SO2 and NOx emissions from the CEM systems will be used. Whereas in the 2006 Typical base case we will analyze the CEM and generate typical summer emissions for when the source is typically operating. The 2006 Actual base case modeling results are compared against the concurrent ambient ozone observations in the model performance evaluation. The 2006 Typical emissions are projected to the future-years for the 2010 and 2020 base case emission scenarios. Modeling results from the 2006 Typical base case emissions scenario are used with results from the future-year emission scenario to project 8-hour ozone Design Values. There is no analogue to the 2006 Actual base case for the future-year emission scenarios. For the WRAP modeling of the 2002 year they also developed Actual and Typical emissions for wildfires because 2002 was an abnormally high year for wildfires in the western U.S. and smoke from wildfires heavily influences visibility at many western Class I areas. However, our preliminary examination of wildfires during the June-July 2006 Denver ozone episode indicates they do not play an important roll in ozone formation in the area, so we would likely just use one set of Actual wildfire emissions for both the 2006 Actual and Typical base case emissions scenarios.

The emissions inventories developed for the Denver 8-hour ozone modeling study will be based on several sources. For the Denver nonattainment area (NAA) the CDPHE/APCD will provide 2006 VOC, NOx and CO emissions. For other pollutants in the Denver NAA (e.g., SO2, NH3 and PM) and emissions outside of the Denver NAA the latest 2002 emissions database, as updated by States and the RPOs, will be projected to 2005/2006. For on-road mobile source emissions in the Denver metropolitan area (DMA), local traffic demand model (TDM) output from the Denver Regional Council of Governments (DRCOG) will be used to generate link-based emissions which will then be gridded for the modeling. For point sources, day-specific hourly NOx and SO2 emissions for sources with Continuous Emissions Monitoring (CEM) systems (e.g., Electrical Generating Units, EGUs) would be used for the 2006 Actual base case simulation used in the model performance evaluation. For the 2006 Typical base case used in the future-year ozone projections the CEM data will be processed to obtain typical 2006 summer emissions for these sources.

Biogenic emissions will be day-specific and based the MM5 model-derived temperatures using the MEGAN biogenic emissions model (Guenther and Wiedinmeyer, 2004). MM5 temperature fields will be reviewed and statistically analyzed for the presence of any daytime temperature bias. If a significant bias exists that cannot be removed through any re-configuration of the model, an alternative means of providing gridded temperature fields from observational analyses will be developed. We would also generate biogenic emissions using the GloBEIS biogenic emissions model that incorporates the BEIS biogenic emissions algorithms that will be used in a sensitivity test. The latest version of MEGAN has not yet been used in a SIP application, whereas GloBEIS has been used extensively for SIPs so would serve as a backup in case issues with the MEGAN biogenic emissions arise.

All emissions, except for on-road mobile source emissions in the DMA will be converted to the Inventory Data Analyzer (IDA) format used by the SMOKE emissions model; the DMA on-road emissions will be generated and gridded using the CONCEPT MV model as discussed below.

5.2.2 Development of CAMx-Ready Emissions Inventories

CAMx-ready emissions will be generated by the SMOKE, CONCEPT and MEGAN suite of emissions models. Table 5-2 summarizes the emissions modeling configuration to be used.

Emissions inventory development for episodic 8-hour ozone modeling must address several source categories including: (a) stationary point sources, (b) area sources, (c) on-road mobile sources, (d) non-road mobile sources, (e) biogenic sources and (f) fire sources. For this analysis, these estimates must be developed for the June-July 2006 modeling period and the 36, 12 and 4 km grids.

CAMx requires two emission input files: (1) low level gridded emissions that are emitted directly into the first layer of the model from sources at the surface with little or no plume rise; and (2) elevated point sources (stacks) with plume rise calculated from stack parameters and meteorological conditions. For ozone modeling alone, hourly emissions are required for NO, NO2, CO, several classes of VOCs and other pollutants as available. The VOC classes used will depend upon the chemical mechanism selected. CAMx will be operated using the CB05 chemical mechanism that will define the VOC classes to be used in the modeling. CAMx will also be configured to provide particulate matter (PM) estimates, as well as visibility and deposition. Thus, additional PM precursor species are needed as emissions input which includes SO2, NH3, SO4, NO3, EC, OMC, other primary $PM_{2.5}$ and coarse PM ($PM_{2.5\text{-}10}$).

A preliminary 36/12/4 km emissions inventory for the June-July 2006 episode will be developed by December 2007 to allow model testing and evaluation. To meet this ambitious schedule the focus will be on the 2006 emissions in the 4 km Colorado domain. The preliminary inventory will use the SMOKE-MOBILE6 module for on-road mobile source emissions everywhere, whereas a refined 2006 on-road mobile source emissions inventory for the DMA will be developed using CONCEPT by February 2008.

Table 5-2. Emissions model configurations.

Emissions Component	Configuration	Details
Model Code	SMOKE Versions 2.3 CONCEPT Version .60 MEGAN	www.cmascenter.org http://www.conceptmodel.org http://bai.acd.ucar.edu/Megan/
Horizontal Grid Mesh	36/12/4 km	
36 km grid	148 x 112 cells	
12 km grid	167 x 92 cells	
4 km grid	119 x 119	
Area Source Emissions	2006 CDPHE/APCD for Denver NAA Projected 2002 RPO outside Denver NAA	SMOKE processing
On-Road Mobile Sources	Denver TDM CONCEPT and MOBILE6 SMOKE-MOBILE6 outside of Denver	CONCEPT processing of link-based TDM data in Denver County HPMS VMT and SMOKE-MOBILE6 outside of Denver
Point Sources	2006 day-specific CEM Projected 2002 RPO outside Denver	Use 2006 day-specific hourly CEM for actual and processed CEM for Typical 2006 emissions
Off-Road Mobile Sources	2006 CDPHE/APCD for Denver NAA Projected 2002 RPO outside Denver NAA	
Emissions Data Sources	2006 CDPHE/APCS for Denver NAA	
	2002 Plan02b WRAP States	Project to 2006
	2002 Base G CENRAP States	Project to 2006
	2002 Base M MRPO States	Project to 2006
	2002 Base G VISTAS States	Project to 2006
	2006 TDM VMT for Denver NAA	Process with CONCEPT-MOBILE6
	2006 HPMS for outside Denver NAA	Process with SMOKE-MOBILE6
	Updated Oil and Gas production emissions	WRAP Phase II inventory for 2005 and western U.S. CDPHE/APCD permits for Colorado (2006) IPAMS 2005 O&G update for eastern Colorado (if available)
	Acid Rain Database for CEM data	Large stationary source NOx and SO2
	WRAP Wind Blown Dust (WBD)	WRAP WBD Model with 2006 MM5 meteorology
	WRAP Ammonia	WRAP NH3 Model with 2006 MM5 meteorology updated with APCD data
Biogenic Sources	MEGAN	
Temporal Adjustments	Seasonal, day, hour	Based on latest collected information
Chemical Speciation	Revised CB05 Chemical Speciation	EPA updated in 2007
Gridding	Spatial Surrogates based on landuse	
Growth and Controls	TBD	2010 and 2020 future years
Quality Assurance	QA Tools in SMOKE and CONCEPT; PAVE plots; Summary reports	

5.2.2.1 Day-Specific On-Road Mobile Source Emissions

The inputs needed to perform on-road mobile sources modeling for the Denver June-July 2006 modeling period on the 36/12/4 km grids include the county-level 2006 vehicle miles traveled (VMT) for the entire modeling domain (36-km grid) and the link-based VMT for the urbanized portion of the Denver area from a travel demand model (TDM). In addition to the link-based VMT data, GIS-based data specifying the locations of the links from transportation modeling are required. Two different emission models will be used to generate on-road mobile source emissions, SMOKE-MOBILE6 for the entire 36/12/4 km modeling domain, and CONCEPT-MOBILE6 for the portion of the DMA that is covered by the link-based TDM VMT data.

5.2.2.1.1 SMOKE On-Road Mobile Emissions for 36/12/4 km Domains

The SMOKE-MOBILE6 emissions model would be used to generate on-road mobile source emissions for the entire 36/12/4 km grids using the 2006 county-level VMT, 2006 MOBILE6 inputs and gridded surrogates.

5.2.2.1.2 CONCEPT On-Road Emissions for the DMA

The Consolidated Community Emissions Processing Tool Motor Vehicle (CONCEPT MV) emissions model will be used to estimate link-level on-road emissions and then grid them for the model input. DRCOG will provide ENVIRON with 2005 TransCAD model output for the DMA. The data provided will be link-specific capacities, volumes, and speeds for a typical weekday for the 10 time periods in each day in the TransCAD model (3 morning peak, 3 afternoon peak, and 4 off-peak time). CONCEPT MV will disaggregate the TDM results for the 10 time periods of the day, and estimate hourly link volumes for weekend days, using total volume temporal profiles by roadway type to be derived by ENVIRON from analysis of Colorado Department of Transportation (CDOT) automated traffic recorder (ATR) monitoring data. CONCEPT MV will then estimate the congested speeds for each link for each hour using the hourly volume/capacity ratios and a formula to be provided by DRCOG. Total volume for each link for each hour will be disaggregated into eight vehicle classes using temporal profiles for VMT mix to be derived by ENVIRON from analysis of CDOT vehicle classification monitoring data as well as a special study of Denver-area roadways VMT mix data recently compiled.

CONCEPT MV is a database application and computing resource intensive. Not all days in the June-July 2006 time period will be run. Rather, ENVIRON will work with CDPHE to define the set of days to be run through CONCEPT MV (e.g., Key high ozone days). The CONCEPT output is gridded CAMx-ready emissions.

5.2.2.2 Episodic Biogenic Source Emissions

Biogenic emissions will be generated using the MEGAN biogenic emissions model. MEGAN uses high resolution GIS data on plant types and biomass loadings and the MM5 surface temperature fields, and solar radiation (modeled or satellite-derived) to develop hourly emissions for biogenic species on the 36/12/4 km grids. MEGAN generates gridded, speciated, temporally allocated emission files. One feature that is included in MEGAN is that it generates biogenic VOC precursor emission species for the new secondary organic aerosol (SOA) module in CAMx.

5.2.2.3 Point Source Emissions

2006 point source emissions for the Denver NAA will be provided by CDPHE/APCD. Outside of the Denver NAA point sources will be developed in two categories – CEM and non-CEM point source emissions. For point sources with continuous emissions monitoring (CEM) data day-specific hourly NOx and SO2 emissions will be used for the 2006 Actual base case emissions scenario. The VOC, CO and PM emissions for point sources with CEM data would be based on the hourly heat input. The locations of the point sources will be converted to the LCP coordinate system used in the modeling. They will be processed by SMOKE to generate the temporally varying (i.e., day-of-week and hour-of-day) speciated emissions needed by CAMx, using standard SMOKE default profiles by source category.

For large point sources with CEM data, we would also developed typical summer emissions for when the source is operating representative of the 2005-2007 planning period that would be used for the 2002 Typical base case. The CAMx results for the 2006 Actual base case are compared against the 2006 measurements in the model performance evaluation, whereas the CAMx results for the 2006 Typical base case are used with the 2010 CAMx results for the 8-hour ozone Design Value projections.

For point source emissions without CEM data, the 2006 emissions inventory will be represented by the existing 2005 point source inventory projected from the RPO 2002 over the 12/36K modeling domain. The portions of the 4 km domain not covered in the Denver NAA will be adjusted to 2006 using Colorado specific projection factors developed in conjunction with CDPHE/APCD

5.2.2.4 Area and Non-Road Source Emissions

County level area source emissions have been taken from the RPO 2002 emissions inventory and projected to 2005 and will be used for the 2006 inventory for the 36/12 km domains. CDPHE/APCD will provide 2006 area and non-road emissions for the Denver NAA. The portions of the 4 km domain not covered in the Denver NAA will be adjusted to 2006 using Colorado specific projection factors developed in conjunction with CDPHE/APCD

The area and non-road sources will be spatial allocated to the grid using an appropriate surrogate distribution (e.g., population for home heating, etc.). In the 4 km domain, specialized spatial surrogates will need to be developed to account for the split of Larimer and Weld counties between the attainment and non-attainment areas. The area sources will be temporally allocated by month and by hour of day using the SMOKE default source-specific temporal allocation factors.

The SMOKE source-specific temporal and CBO5 speciation allocation profiles will be used.

5.2.2.5 Wildfires, Prescribed Burns, Agricultural Burns

If there are indications of any fires present near the Denver area that may affect ozone air quality during June-July 2006 they will be accounted for in the model as information, resources and time are available. We have performed an initial survey of the reporting of fires during the modeling period as documented on the National Fire and Aviation Management website (FAMWEB; http://fam.nwcg.gov/fam-web/). The occurrence of reported fires within the 4 km Colorado grid by 20 day increments during the modeling period are shown in Figure 5-1. The only fire reported near the DMA during the June-July 2006 modeling period was in southwestern Jefferson County during the first quarter of the modeling period (May 25-June 15). This period includes one of the nine 8-hour ozone exceedance days during the modeling period. This exceedance day (June 12, 2006) was a minor exceedance day with measured exceedances occurring only at the Fort Collins West monitor far north of the reported fire that is southwest of the DMA. This preliminary analysis suggests that emissions from fires did not play a pivotal role in the 2006 summer's ozone exceedances in the DMA and vicinity. Further analysis is needed to verify this, but if true then emissions from fires may not need to be modeled.

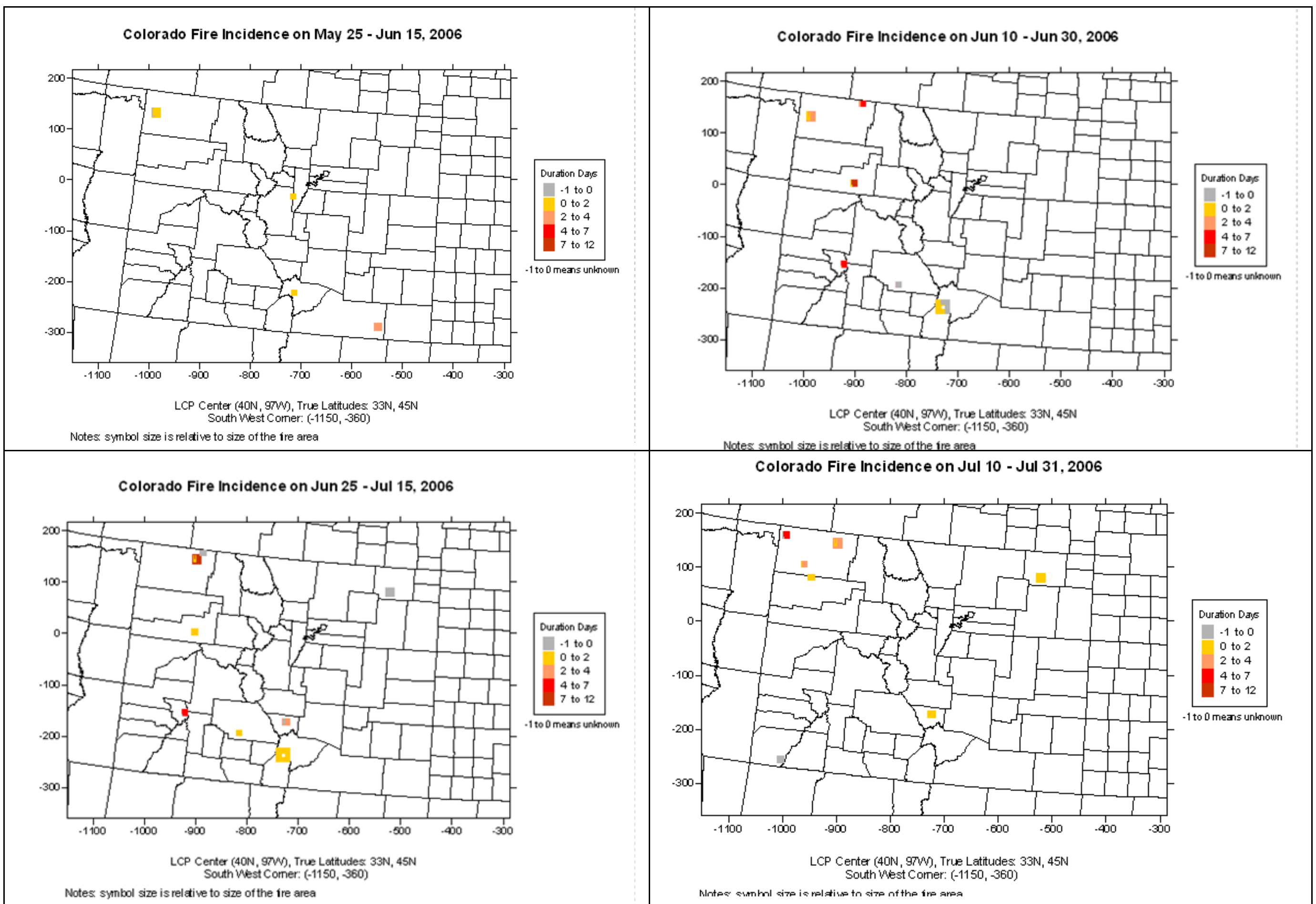


Figure 5-1. Occurrence of reported wildfires in Colorado during the June-July 2006 modeling period broken down by May 25-June 15 (top left), June 10-30 (top right), June 25-July 15 (bottom left) and July 10-July 31, 2006 (bottom right).

5.2.2.6 QA/QC and Emissions Merging

The emissions will be processed by major source category in several different "streams", including area sources, on-road mobile sources, non-road mobile sources, biogenic sources, non-CEM point sources, CEM point sources using day-specific hourly emissions (Actual), CEM sources using average emissions (Typical) and, as available, emissions from fires. Separate Quality Assurance (QA) and Quality Control (QC) will be performed for each stream of emissions processing and in each step. SMOKE includes advanced quality assurance features that include error logs when emissions are dropped or added. In addition, we will generate visual displays that include:

- Spatial plots of the hourly emissions for each major species (e.g., NOx, VOC, some speciated VOC, SO2, NH3, PM and CO);
- Vertical average emissions plots for major species and each of the grids;
- Diurnal plots of total emissions by major species; and
- Summary tables of emissions for major species for each grid and by major source category.

This QA information will be examined against the original point and area source data and summarized in an overall QA/QC assessment.

Scripts to perform the emissions merging of the appropriate biogenic, on-road, non-road, area, low-level, fire, and point emission files will be written to generate the CAMx-ready two-dimensional day-specific hourly speciated gridded emission inputs. The point source and, as available elevated fire, emissions would be processed into the day-specific hourly speciated emissions in the CAMx-ready point source format.

The resultant CAMx model-ready emissions will be subjected to a final QA using spatial maps, vertical plots and diurnal plots to assure that: (1) the emissions were merged properly; (2) CAMx inputs contain the same total emissions; and (3) to provide additional QA/QC information.

5.2.3 Use of the Plume-in-Grid (PiG) Subgrid-Scale Plume Treatment

The Plume-in-Grid (PiG) sub-model treats the early plume chemistry and dynamics of emissions from point sources and then releases the emissions into the grid model farther downwind at such time that the plume is adequately resolved by the grid. There are currently two PiG options in the CAMx model:

- GREASD PiG: The Greatly Reduced Execution and Simplified Dynamics (GREASD) Plume-in-Grid (PiG) module treats the early plume dynamics and inorganic NOx chemistry, and releases the emissions from the PiG to the grid model when organic chemistry starts being important; and
- IRON PiG: The Incremental Reactions for Organics and NOx PiG module treats the full chemistry at all downwind distances.

The GREASD PiG was designed for large NOx point source plumes, where the early evolution of the plume is dominated by NOx and inorganic chemistry. Because of the high NOx in these plumes, the mass they carry are typically released to the grid model at the time that organic chemistry becomes important.

The IRON PiG uses full chemistry and is appropriate for both NOx and VOC plumes. Currently the CAMx model can only use one PiG module in each run (i.e., it cannot run point source X with GREASD PiG and point source Y with IRON PiG in the same run).

Large NOx plumes will be selected for treatment by the subgrid-scale PiG module. The selection of which sources to be treated by the PiG module will be made after a review of the inventory. Tests may be conducted to determine the sensitivity of the ozone estimates in the Denver area to the use of the different PiG modules.

5.2.4 Products of the Emissions Inventory Development Process

In addition to the CAMx-ready input files generated for each hour of all days modeled in the Denver June-July 2006 modeling period, a number of quality assurance (QA) files will be prepared and used to check for gross errors in the emissions inputs. Importing the model-ready emissions into PAVE and looking at both the spatial and temporal distribution of the emission provides insight into the quality and accuracy of the emissions inputs.

- Visualizing the model-ready emissions with the scale of the plots set to a very low value, we can determine whether there are areas omitted from the raw inventory or if emissions sources are erroneously located in water cells;
- Spot-checking the holiday emissions files to confirm that they are temporally allocated like Sundays;
- Producing pie charts emission summaries that highlight the contribution of each emissions source component (e.g. nonroad mobile);
- Normalizing the emissions by population for each state will illustrate where the inventories may be deficient and provide a reality check of the inventories.

State inventory summaries prepared prior to the emissions processing will be used to compare against SMOKE output report totals generated after each major step of the emissions generation process. To check the chemical speciation of the emissions to CB05 species, we will compare reports generated with SMOKE to target these specific areas of the processing. For speciation, the inventory state import totals will be compared against the same state totals with the speciation matrix applied.

The quantitative QA analyses often reveal significant deficiencies in the input data or the model setup. It may become necessary to tailor these procedures to track down the source of each major problem. As such, one can only outline the basic quantitative QA steps that we will perform in an attempt to reveal the underlying problems with the inventories or processing. Following are some of the reports that may be generated to review the processed emissions:

- State and county inventory totals for each source category.
- State and county totals after spatial allocation for each source category.

- State and county totals by day after temporal allocation for each source category for representative days.
- State and county totals by model species after chemical speciation for each source category.
- State and county model-ready totals (after spatial allocation, temporal allocation, and chemical speciation) for each source category and for all source categories combined.
- If elevated source selection is chosen by user, the report indicating which sources have been selected as elevated and plume-in-grid will be included.
- Totals by source category code (SCC) from the inventory for area, mobile, and point sources.
- Totals by state and SCC from the inventory for area, mobile, and point sources.
- Totals by county and SCC from the inventory for area, mobile, and point sources.
- Totals by SCC and spatial surrogates code for area and mobile sources.
- Totals by speciation profile code for area, mobile, and point sources.
- Totals by speciation profile code and SCC for area, mobile, and point sources.
- Totals by monthly temporal profile code for area, mobile, and point sources.
- Totals by monthly temporal profile code and SCC for area, mobile, and point sources.
- Totals by weekly temporal profile code for area, mobile, and point sources.
- Totals by weekly temporal profile code and SCC for area, mobile, and point sources.
- Totals by diurnal temporal profile code for area, mobile, and point sources.
- Totals by diurnal temporal profile code and SCC for area, mobile, and point sources.
- PAVE plots of gridded inventory pollutants for all pollutants for area, mobile, and point sources.

5.2.5 Future-Year Emissions Modeling

Future-year emission inputs will be generated by SMOKE by projecting the current year (e.g., 2006) inventory using growth and control factors. Growth and control factors representative of Colorado and the DMA would be determine with input from the RAQC, CDPHE/APCD and modeling team.

5.3 Photochemical Modeling Inputs

5.3.1 CAMx Science Configuration and Input Configuration

This section describes the model configuration and science options to be used in the Denver 8-hour ozone modeling effort. Table 5-3 summarizes the CAMx configuration to be used. The latest version of CAMx (Version 4.5) will be used in the Denver modeling. The model will be configured to predict both ozone and PM species.

As indicated in the CAMx model setup defined in Table 5-3, three grids will be employed. CAMx would be initially run for the 2006 base case on the 36 km continental U.S. grid for the May 25 through July 31, 2006 period and output three-dimensional concentrations of all modeled species. The 36 km continental U.S., CAMx outputs would be processed to define hourly initial concentrations (ICs) for June 1, 2006 and boundary conditions (BCs) for June 1 through July 31, 2006 period and the 12 km grid. CAMx would then be run for the 2006 Actual base case on the 12/4 km grid using two-way interactive grid nesting and the IC/BC from the 36 km CAMx simulation. The PPM advection solver will be used along with the spatially varying (Smagorinsky) horizontal diffusion approach. K-theory will be used for vertical diffusion.

The CB05 gas-phase chemical mechanism is selected because it includes the very latest chemical kinetic rates and represents improvements over the CBM-IV and SAPRC99 chemical mechanisms. Additional CAMx inputs will be as follows:

Meteorological Inputs: The MM5-derived meteorological fields will be prepared for CAMx using MM5CAMx. Several alternative vertical diffusivity options will be generated for CAMx input and evaluated in sensitivity tests, as described earlier.

Initial/Boundary Conditions: The IC/BC for the 36 km continental U.S. simulation would be based on the latest available information. Currently the RPOs are using IC/BC for the same domain based on a 2002 GEOS-CHEM global chemistry model simulation. We are aware of the availability of 2006 MOZART global model output that may be used to define BCs for the outer 36 km modeling domain. A processor will need to be written to interpolate from the MOZART horizontal and vertical coordinate system to the CAMx LCP coordinate system and map the MOZART chemical species to the CB05 chemical mechanism.

Photolysis Rates: The modeling team will prepare the photolysis inputs as well as albedo/haze/ozone/snow inputs for CAMx based on Total Ozone Mapping Spectrometer (TOMS) data. For CAMx the TUV processor will be used. If there are periods of more than a couple of days where daily TOMS data are unavailable, monthly average TOMS data will be used.

Landuse: The team will generate landuse fields based on USGS GIRAS data and local-specific land use data available from the APCD.

Spin-Up Initialization: Five days of spin up will be specified (May 25-30, 2006) using the 36 km continental U.S. configuration before the first day of the modeling period (June 1, 2006). The first 8-hour ozone exceedance day in the Denver area is June 12 which gives us 17 days of spin up on the 36 km grid and 11 days of spin up on the 12/4 km grid, which should be more than sufficient.

Table 5-3. CAMx (Version 4.5) model configuration.

Science Options	Configuration	Details
Model Code	CAMx (v4.5) – 2007 Release	Available at: www.camx.com
Horizontal Grid Mesh	36/12/4 km	
36 km grid	148 x 112 cells	One-way nest with 12 km grid
12 km grid	167 x 92 cells	BCs from 36 km run
4 km grid	119 x 119	Two-way nesting with 12/4 km grids
Vertical Grid Mesh	19 vertical layers, defined by MM5	Layer 1 thickness ~ 35 m
Grid Interaction	36/12 km one-way and 12/4 km two-way nesting	
Initial Conditions	Default – 5 day spin-up on 36 km grid	
Boundary Conditions	36 km TBD; 12 km from 36 km simulation	Monthly average diurnally varying 2002 GEOS-CHEM BCs available for 36 km grid
Emissions		
Baseline Emissions Processing	SMOKE	
Sub-grid-scale Plumes	Plume-in-Grid for major NOx sources and potentially VOC sources	GREASD-PiG NOx chemistry plume model or IRON-PiG full chemistry plume model
Chemistry		
Gas Phase Chemistry	CB05	Latest chemical reactions and kinetic rates
Meteorological Processor	MM5CAMx	Compatible with CAMx v4.5
Horizontal Diffusion	Spatially varying	K-theory with Kh grid size dependence
Vertical Diffusion	Kv (O'Brien '70, CMAQ, TKE methods)	Sensitivity tests to Kz methods
Diffusivity Lower Limit	Kz-min = 0.1 to 1.0 m^2/s	Run MM5CAMx with Kz_min = 0.1 m^2/s; sensitivity tests for Kz_min
Deposition Schemes		
Dry Deposition	Wesley resistance scheme	Wesley (1989)
Wet Deposition	CAMx-specific formulation	rain/snow/graupel
Numerics		
Gas Phase Chemistry Solver	Chemical Mechanism Compiler-- Fast Solver	ENVIRON (2006)
Vertical Advection Scheme	Fully implicit scheme	
Horizontal Advection Scheme	Piecewise Parabolic Method (PPM) scheme	
Integration Time Step	Wind speed dependent	~0.5-1 min (4-km), 1-5 min (12-km), 5-15 min (36-km)

6.0 MODEL PERFORMANCE EVALUATION

This chapter describes the model performance evaluation from which to establish reliable CAMx 8-hour ozone modeling for the Denver area. In general terms, this process consists of the following cycle:

- Exercise the modeling system for the base case, attempting to replicate the time and space behavior of the observed 1-hour and 8-hour ozone concentration fields as well as concentrations of precursor and product species;
- Evaluate the model's fidelity in simulating ozone and precursor/product species using a two-step process consisting of: (a) an initial "screening model performance evaluation" (SMPE) process, and if the modeling results pass the screening analysis, (b) a "refined model performance evaluation" (RMPE) consisting of progressively more stressful testing procedures involving multi-species, multi-scale surface and aloft model performance evaluation (MPE);
- Identify sources of error and/or compensating biases, through evaluation of preprocessor models (MM5, SMOKE, CONCEPT, MEGAN), air quality model inputs, concentrations aloft, mass budgets and conservation, process analysis, etc;
- Through a documented process of diagnostic and sensitivity investigation, pinpoint and correct the performance problems via model refinement, additional data collection and/or analysis, or theoretical considerations;
- Re-run the model for the base case and re-evaluate performance until adequate, justifiable performance is achieved or the modeling period is declared unsuited for further use based on documented performance problems.

To an extent, some or all of these steps will be taken by the modeling team for the June-July 2006 period ideally culminating in a modeling database demonstrated to exhibit sufficiently minimal bias and error that they may be used reliably to evaluate 8-hour ozone control strategies and to perform an 8-hour ozone attainment demonstration. In the following subsection, we briefly identify the steps that will be taken by the modeling team in constructing and evaluating the CAMx base cases for 8-hour ozone SIP development in Denver.

6.1 Establishing Base Case CAMx Simulations for Denver

6.1.1 Setting Up and Exercising CAMx Base Cases

The modeling team will select the final model configurations for the CAMx base case simulation for June-July 2006 (see Chapter 5). The modeling team will define the recommended final model configurations based on results from the initial configuration runs (see Tables 5-1 through 5-4) and a series of model sensitivity tests. The series of model sensitivity tests will be conducted for the July 20-30, 2006 period on the 4 km grid to identify the optimal MM5 meteorological, SMOKE/CONCEPT/MEGAN emissions and CAMx air quality model configurations for simulating ozone formation in the Denver area.

The optimal model configurations will be identified based on the following factors:

- Model performance obtained using the initial model configurations and input data;
- Model performance for base case sensitivity tests;
- The modeling team's knowledge of the CAMx model configurations and associated attributes;
- Experience performing sensitivity tests and model performance evaluation for the Denver 8-hour ozone EAC SIP, New Mexico 8-hour ozone EAC SIP, FCAQTF CAMx, BLM EIS CAMx and CMAQ, WRAP, CENRAP, VISTAS, MRPO, and numerous other modeling studies carried out by the modeling team; and
- Comments from RAQC, APCD, EPA, Stakeholders and other participants.

The objective in identifying optimum model configurations is to obtain the best performance for the right reasons consistent with sound science and EPA guidance. Sometimes, decisions must be made that trade off better/poorer model performance for one pollutant against another. For example, although the focus of the model evaluation is on ozone and ozone precursor and product species, we will also evaluate the model for $PM_{2.5}$, PM species (e.g., SO4, NO3, NH4, EC, OMC, Soil and CM), deposition and visibility but the primary focus will be for ozone. These factors will be considered and potential issues discussed among the modeling team, RAQC, APCD, EPA and others. Based on the analysis and comments from RAQC, APCD, EPA and other interested parties, the modeling team will select the final model configurations.

6.1.2 Use of Sensitivity, Source Apportionment, and Related Diagnostic Probing Tools

The Denver ozone study may utilize several diagnostic and probing tools to further test and understand the CAMx base case ozone simulations. The use of these tools is discussed below.

Traditional Sensitivity Testing: Traditional sensitivity testing will be performed using the CAMx model. Once each model is operating properly for each base case, sensitivity runs may be performed to explore response to emissions changes as well as changes in key input parameters. These sensitivity runs serve two purposes:

- To assist in improving model performance;
- Aid in helping to define appropriate emissions control scenarios; and
- Provide episode-specific model uncertainty information that may be used later in "Weight of Evidence" analyses in support of the 8-hour ozone attainment demonstration.

Ozone Source Apportionment: Focused use of ozone source apportionment technology (OSAT) for selected episodes may be employed to better understand model response and to aid in the design of control strategies. Source apportionment modeling will be conducted for subsequent stages of the Denver modeling study for the 2010 emission scenario and these calculations will help to:

- Assess the contribution of sources in the Denver NAA, Colorado and surrounding areas to ozone concentrations at key Denver receptor locations; and

- Identify the particular source categories that may contribute the most to elevated 8-hour ozone concentrations in the Denver NAA.

DDM Sensitivity Modeling: Another type of sensitivity that may be performed entails the use of the Direct Decoupled Method (DDM) technology in CAMx. DDM may be set up and exercised for a potion of the Denver modeling period to produce a numerically intensive, direct sensitivity/uncertainty analysis. DDM can provide information on the sensitivity of ozone to model inputs (e.g., IC, BC, specific emissions). For example, it was used in the Houston area to identify where locations of potential highly reactive VOC emissions would be that could explain the rapid rise in ozone at a particular time and location (i.e., assuming that VOC emissions are missing from the inventory, what emissions locations would best explain observed high ozone levels?).

Process Analysis: Process Analysis is a tool in CAMx to extract additional information about the various physical and chemical processes in the model that produced the ozone concentrations. Information on VOC-limited versus NOx-limited ozone formation, importance of local production versus entrainment of ozone aloft and identification of the contributions of individual VOC species to ozone formation are the types of information that can be obtained with Process Analysis. It can be a powerful tool for diagnosing the causes of poor model performance.

For the 2006 base case modeling and model performance evaluation, only traditional sensitivity tests will be utilized to help improve model performance due to resource and time constraints. Source apportionment modeling will be use with the 2010 modeling to assist in control strategy development.

6.2 Evaluation of CAMx Base Cases for the Denver Region

This section describes the procedures for evaluating the performance of the meteorological and photochemical models using the available aerometric data sets for the Denver ozone episodes.

6.2.1 Overview

Model performance evaluation (MPE) is the process of testing a model's ability to accurately estimate 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. Below we summarize the philosophy and objectives that will govern the evaluation of the MM5, SMOKE/CONCEPT/MEGAN and CAMx models for the Denver 8-hour ozone application. Specific evaluation methods are identified that will be employed to judge the suitability of the meteorological and air quality 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; 2005a; 2007) for 1-hour and 8-hour ozone attainment demonstration modeling.

We begin by establishing a framework for assessing whether the SMOKE/CONCEPT/MEGAN/MM5/CAMx modeling system (i.e., the emissions, meteorological and chemical dispersion models and their supporting data sets) perform with sufficient reliability to justify their use in developing 8-hour ozone control strategies for the Denver nonattainment area. The models' 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 SMOKE, CONCEPT and MEGAN 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 for the reasons identified by Roth et al. (2005). This includes EPA's ozone 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 simulating air quality in the Denver Front Range region; 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.

A rigorous ozone model evaluation in typical regulatory applications consists of two components. The *operational evaluation* entails an assessment of the model's ability to correctly estimate surface meteorological or air quality variables largely independent of whether the actual process descriptions in the model are accurate. The operational evaluation essentially tests whether the predicted surface meteorological and air quality fields are reasonable, consistent and agree adequately with routinely available observations. In this study, the operational evaluations focus on the various model's reliability in reproducing hourly-average surface wind speed, wind direction, temperature, mixing ratio and ozone and precursor concentrations within and nearby the Denver area. However, we will also evaluate the modeling system for meteorological variables, ozone, PM mass, PM species and other species concentrations, deposition and visibility across the Colorado 4 km and larger Western U.S. 12 km grid.

The *scientific evaluation* addresses the realism of the meteorological and air quality processes simulated by the models through testing the model as an entire system (i.e., not merely focusing on surface wind, temperature or ozone 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 decisions based on model usage. Ideally, the scientific evaluation consists of a series of diagnostic and mechanistic tests aimed at: (a) examining the existence of compensatory errors, (b) determining the causes of failure of a flawed model, (c) stressing a model to ensure failure if indeed the model is flawed, and (d) providing additional insight into model performance beyond that supplied through routine, operational evaluation procedures.

Practically, a rigorous scientific evaluation is seldom feasible due to the absence of the specific measurements needed to test the process modules (e.g., soil moisture, Reynold's stress measurements, PBL heights, trace gas species, and so on). Accordingly, the overall model performance evaluation in this study is constrained mainly to operational testing of the MM5 models' primary meteorological outputs (i.e., wind speed, wind direction, temperature, and moisture) and the CAMx model's predictions of ozone, NOx, CO and potentially VOC, PM mass, PM species, visibility and deposition. However, some components of the scientific evaluation of the air quality model are possible through examination of ground-level and aloft primary and product species and species ratios. In addition, corroborative analyses involving joint analysis of emissions inventory estimates, air quality model predictions and ambient measurements add to the scientific evaluation.

6.2.2 Meteorological Model Evaluation Methodology

Meteorological inputs required by the CAMx model include hourly estimates of the three-dimensional distribution of winds, temperatures, mixing ratio, pressure, clouds, and precipitation, 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 the surface and aloft meteorological fields for the Denver ozone modeling episodes.

6.2.2.1 Components of the Denver 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, has 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. Note that further develop of the MM5 model has been stopped and development efforts are now focused on Weather Research Forecast (WRF) meteorological model.

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 these types of measurements may be limited over Denver during the modeling episode, a meaningful scientific evaluation of the MM5 may not be possible in this study. However, if the operational evaluation presented in subsequent chapters is performed thoroughly, they are expected to be sufficient to serve as the basis for judging whether the model is operating with sufficient reliability over the Denver domain to be used in the photochemical modeling portion of this study.

6.2.2.2 Data Supporting Meteorological Model Evaluation

Hourly surface meteorological observations will be obtained from the National Center for Atmospheric Research and other sources to support the evaluation of MM5 near-surface temperature, water vapor, and wind speed fields. The specific NCAR data set used for this purpose is 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. These data sets will be collected in performing the Denver MM5 model evaluation. For precipitation the Climate Prediction Center historical archives will be used.

6.2.2.3 Evaluation Tools

The primary tool used for evaluating the MM5 meteorological model in air quality modeling study is the METSTAT program developed by ENVIRON. METSTAT calculates a suite of model performance statistics using surface wind speed, wind direction, temperature and water vapor mixing ratio for use specified subdomains. Tables 6-1 and 6-2 list some of the model performance evaluation metrics to be used in evaluating the MM5 model. We will use both regional as well as local subdomains in the METSTAT analysis. Regional domains would include those used by WRAP (Kemball-Cook et al., 2005), CENRAP (Johnson, 2007) and others so that the Denver MM5 performance can be compared with other MM5 performance in the same subdomains to help put the results into context and against meteorological model performance benchmarks (Emery, Tai and Yarwood, 2001). Local domains would include the Denver area and possibly even more refined subdomains. The evaluation of the MM5 aloft meteorological estimates with upper-air observations would be accomplished using the RAOBS program developed by the State of Iowa (Johnson, 2007). Additional comparisons of the spatial patterns of precipitation and clouds may also be made using satellite and radar-based data.

6.2.3 Photochemical Model Evaluation Methodology

The CAMx performance evaluations will follow the procedures recommended in the EPA photochemical modeling guidance documents (EPA, 1991; 1999; 2005a; 2007). 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 available precursor and product species, comparisons of pollutant ratios and groupings, comparison against PM species, deposition and visibility). That is, the specific two-step ozone evaluation process is:

- An initial "screening model performance evaluation" (SMPE) process, and if the modeling results pass the screening analysis;
- A "refined model performance evaluation" (RMPE) consisting of progressively more stressful testing procedure involving multi-species, multi-scale surface and aloft MPE;

Below we describe how this evaluation will be conducted. The formal procedures outlined in EPA recent 8-hour modeling guidance (EPA, 2007) will be used to evaluate CAMx for the Denver modeling episode. The modeling team will consider 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 as available; 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 fully support all six of these analyses. This may not be possible with the current air quality data collected in the Denver area, particularly in regards to precursor measurements, since limited measurements were conducted in this area during the proposed modeling period. During 2006 there were two routine monitoring sites collected NO2 measurements (Denver CAMP and Welby) and 13 monitors for CO.

We are aware of three "field study" campaigns in the general Denver area during 2006 that may provide additional data to evaluate the modeling system:

- The CDPHE/APCD collected VOC samples during 2006 that will assist in evaluating this important ozone precursor. Most VOC samples were collected in the morning (6-9am MDT) with samples for the following sites available during some days of the June-July 2006 modeling episode:
  - CAMP
  - Welby
  - Fort Lupton
  - Platteville
  - Rocky Flats North
  - Fort Collins West
- During portions of 2006, NOAA launched daily ozonesondes at numerous sites throughout the U.S., including Boulder. The ozonesonde measurements will provide valuable information on the vertical structure of ozone concentrations, including the potential identification of an ozone reservoir aloft.

- Finally, the NPS and CDPHE collected special measurements as part of the ROMANS study during 2006.

The modeling team is in the process of acquiring this special study so they can assess their own usefulness in the Denver ozone study model performance evaluation. 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 of the CAMx base case ozone predictions (i.e., the SMPE) will be performed for the initial base case and each sensitivity test in an attempt to identify obviously flawed model simulations and to implement and identify improvements to the model input files in a logical, defensible manner. The screening SMPE will employ some of the more appropriate ozone performance statistics and plots listed in Table 6-3. Examples of the types of graphical displays that may be helpful in the SMPE include the following for both 1-hour and 8-hour ozone concentrations:

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

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 will 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 and discussed with key participants (e.g., RAQC, APCD, EPA);
- 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; and
- 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 screening of the CAMx ozone results does not reveal obvious flaws, the refined model performance evaluation will be carried out. If significant performance issues are uncovered in the SMPE, further model diagnosis and quality assurance of the input files and related model performance improvement analyses will be performed. That is, the full refined model performance evaluation will not be carried out on obviously flawed model simulations as it would be wasteful of project resources and schedule.

Assuming the SMPE is satisfactory, the formal operational evaluation in the RMPE will commence. First, the graphical displays utilized previously for ozone may be generated for NOx, VOC, and key product species (e.g., HNOx, PAN) as available. Note that model performance for VOC and many product species may be limited since there are little relevant ambient measurements collected in the Denver area. But even so, the graphical displays for ozone precursor and product species will be examined for obvious flaws that may be readily apparent even in the absence of measurements. Should these be detected, the model diagnosis and performance improvement efforts may be needed to fully identify, correct (if possible) and document the noted problems. Table 6-4 lists performance evaluation techniques for a RMPE.

Second, diagnostic analysis and testing, including a limited number of model sensitivity and/or uncertainty simulations, will likely be performed to help elucidate model performance and response to changes in key inputs. Sensitivity analysis, often an important component of the evaluation process, will be performed to aid in understanding the air quality model's response to key input parameter uncertainties. They provide evidence that the model is responding as expected relative to local understanding of the conditions leading to high ozone (i.e., conceptual models). The extent to which sensitivity simulations with CAMx will be needed can only be assessed after the initial model evaluations are performed. With the advent more sophisticated one-atmosphere models, certain sensitivity runs historically carried out older models (e.g., UAM family) are no longer feasible, needed, or appropriate (e.g., zero IC/BC or zero-emissions runs). Other, more insightful and physically meaningful experiments are used (e.g., NOx and VOC emission changes, vertical eddy diffusivity and grid changes, alternative chemistry mechanisms, alternative meteorological realizations, etc.).
Emission sensitivity tests are particularly relevant as they provide: (1) a reality check that the model is responding as expected; (2) information on which emission source components are important; and (3) initial quantification of potential impacts of controls.

Sensitivity experiments will be conduced as part of the CAMx model performance evaluation analysis to assist in identifying the optimal model configurations for simulating ozone formation in the Denver area. As noted previously, in order to maximize the potential number of sensitivity tests they will focus on the July 20-30, 2006 period and the 4 km grid. However, performing sensitivity tests for other model periods may also be performed and the final model simulations will be for the full June-July, 2006 modeling period on the 36/12/4 km modeling grids. The potential need for and nature of these simulations would be discussed among the modeling team and RAQC/APCD after the operational evaluation results have been reviewed.

6.2.4 Available Aerometric Data for the Evaluations

Limited concentration measurements and meteorological parameters are available for the Denver area. These will be used to the fullest extent possible in the evaluation of the MM5 and CAMx models. Table 4-4 presented previously discusses the availability of gaseous and particle air quality measurements from routine monitoring networks operating in the U.S. Examples of available air quality data available for the evaluation are summarized as follows:

AIRS Surface Air Quality Data: Data files containing hourly-averaged concentration measurements at a wide variety of state and EPA monitoring networks are available in the AIRS/AQS database. These data sets will be reformatted for use in the model evaluation software. Typical surface measurements at the ground level routine AIRS monitoring stations include ozone, NO_2, NO_x and CO. Figure 4-2 and Table 4-2 presented previous displays the ozone monitoring sites within and near the Denver NAA.

IMPROVE Monitoring Network: The National Park Service (NPS) operates an IMPROVE monitor at Rocky Mountain National Park (RMNP) that measures PM mass and $PM_{2.5}$ speciation

Other Monitoring Networks: There may be special air quality measurements collected by private industry or public agencies in the area. These include the CDPHE/APCD VOC sampling, NOAA ozonesonde and ROMANS studies discussed earlier. The modeling team will work with the RAQC and APCD to obtain as much data as are available for the model performance evaluation.

Table 6-1. Statistical measures and graphical displays used 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

Statistical Measure	Graphical Display
	temperatures
Mean bias in hourly surface temperature	Scatterplot of daily maximum observed 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 6-2. Statistical measures and graphical displays used 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 6-3. Statistical measures and graphical displays for 1-hour and 8-hour ozone concentrations to be used in the screening model performance evaluation (SMPE) of CAMx surface ozone concentrations.

Statistical Measure on 36/12/4 km grids	Graphical Display on all grids
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	
Variance in hourly concentrations	

Table 6-4. Statistical measures and graphical displays for 1-hour and 8-hour ozone, VOCs, NOx, and indicator species and indicator species. Ratios to be used in the refined model performance evaluation (RMPE) involving multi-species, multi-scale evaluation of CAMx surface and aloft concentrations.

Statistical Measure on 36/12/4 km grids	Graphical Display on all grids
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	
Variance in hourly concentrations	
Mean, maximum, minimum, standard deviation, bias and error of observed and modeled aloft concentrations (e.g., ozone, NO_x) along individual aircraft paths	Modeled and observed time series of ozone and NO_x concentrations along individual aircraft flight paths

7.0 FUTURE YEAR MODELING

This chapter discusses the future year modeling procedures to be performed by the modeling team for the Denver June through July 2006 ozone modeling period for use in 8-hour hour ozone attainment demonstration modeling. Note that the modeling team, RAQC and APCD are still developing the approach for performing future-year emission projections and more details will be reported in the future.

7.1 Future Year to be Simulated

Denver is expected to be designated as a Marginal 8-hour ozone nonattainment area under Subpart 2 of the Clean Air Act Amendments (CAAA) in November 2007 and will be required to attain the current 8-hour ozone standard by 2010. Thus, the 2010 future year will be modeled for the attainment demonstration.

7.2 Future Year Growth and Controls

Several RPOs, including WRAP, CENRAP, VISTAS, WRAP and the MRPO, have performed refined future year modeling inventories for 2018 and some have also modeled 2009 (VISTAS and MRPO) and even 2012 (MRPO). EPA has developed future year inventories for 2010 and 2015 as part of their CAIR/CAMR analysis. These regional growth and control factors will be the starting point for the 2010 future year inventory development augmented by local data as available.

7.2.1 Regional Growth and Control Factors

Coordinating with the WRAP, CENRAP, MRPO, VISTAS, MANE-VU and EPA, the modeling team will review and refine national and regional growth factors, MOBILE6 input files, and control program reduction estimates that are consistent with Denver's 2010 future year base case for the attainment demonstration.

The files prepared will include all federally promulgated rules for the 36 km regional-scale domain and will be largely based on data prepared by the RPOs (e.g., WRAP, CENRAP, MRPO and VISTAS), States (e.g., Colorado) and EPA. This information is based on the latest publicly available information from EPA's federal rulemaking process and at the time of this writing are deemed to be the most recent information available on the topic. Each reviewed rule and regulation found applicable to the U.S. modeling domain relevant to ozone abatement will be documented with cite, geographic coverage, source categories of impact, and associated and expected emission reduction potential. Additional synchronization with EPA and WRAP's sister RPOs will be conducted to ensure consistent, if not comparable, application of these programs.

Using summary files prepared to present this information in an easily reviewable format, the modeling team will contact individually identified or otherwise interested regional representatives to solicit comment on the originally presented growth and control factors. Upon review and comment of these factors, the team will revise the regional growth and control factors consistent with the comments collected. The control factor lists will then be compared to the base year emission inventory to determine which, if any, of these programs may already be accounted for in the emission estimates. The factors will be converted to create a complete set of growth and control packets allowing the generation of future year controlled emissions.

7.2.2 Local Growth and Control Factors

The modeling team will work with the RAQC, CDPHE/APCD and others to develop local emissions inventory for the DMA representation of 2010. TDM output of 2010 link-based VMT, speeds, fleet distributions, etc. will be used with the MOBILE6 2010 emissions factor in the CONCEPT model to generate 2010 on-road mobile source emissions for the DMA. The EPA NONROAD model along with the SMOKE emissions model will be used to generate 2010 non-road emissions for the DMA. Area and point sources will be projected to 2010 using growth and control factors reviewed by RAQC and APCD. 2010 oil and gas production emissions will be generated for the area.

7.3 Future Model–Ready Emissions Inventory Development and QA

Future year emissions will be processed into the gridded speciated hourly three-dimensional emissions inputs for the CAMx photochemical model using the SMOKE emissions model for all sources except on-road mobile sources in the DMA for which the CONCEPT model will be utilized. The same MEGAN (or alternative) biogenic emissions as used in the 2006 base year modeling will be used for the future-year modeling. This assumes that the same land use and biomass distribution as used in the base case emissions would exist in the future-year emission scenarios. The effects of changes in Denver landuse (growth), agriculture, deforestation, etc. between the current and future-year would not be accounted for. We are looking at this issue more closely to see whether changes in land use can be accounted for in the future year modeling. Typical-year EGU and fire emissions (if fires were included in the base year emissions scenario) would also be used in the future-year.

Similar QA/QC will be performed on the future year model-ready emissions inventories as were utilized in checking the base year datasets described in Chapter 5. Standard inventory assessment methods will be employed to generate the future year emissions data including, but not limited to: (a) visualizing the model-ready emissions graphically, (b) spot-checking the holiday emissions files to confirm that they are temporally allocated like Sundays, (c) producing pie charts emission summaries for each source category, (d) normalizing the emissions by population for each state to reveal where the future year inventories may be suspect and (e) spot-checks of the vertical allocation of point sources using PAVE. The additional QA analyses and reports that we may find particularly useful for the future year emissions files are given in Section 5.2.4.

7.4 Future Year Baseline Air Quality Simulations

The Denver future-year modeling will use the MM5 meteorological conditions developed for the Denver June-July 2006 modeling period. That is, the meteorological conditions for the future-year are assumed to be the same as for the 2006 base year ozone episode. This will allow for the comparison of the changes in 8-hour ozone concentrations in the study area from the current to future-year due to changes in emissions only. This means that the effects of inter-annual variability, land use variations and climatic variations will not be accounted for in the future-year meteorological inputs. Several other decisions concerning the future-year to be modeled, model(s) to be used, and modifications to the model inputs to reflect future years, need to be made, as described below.

7.4.1 Future-Year Initial and Boundary Conditions

The same initial conditions as used in the base year would be used in the future-year modeling. Because a minimum 5-day spin up period is being used on the 36 km grid, initial conditions should have minimal if any influence on the model estimated concentrations.

2010 boundary conditions (BCs) for the 2010 CAMx 36 km simulations will be consistent with those developed for the 2006 base case modeling discussed in Chapter 5. The exact definition of the 2010 BCs for the 36 km domain cannot be specified at this time, but because the relative changes in the modeling results between 2006 and 2010 are used then the BCs for the two years must be consistent.

7.4.2 Other Future-Year Modeling Inputs

All other future-year CAMx modeling inputs will be identical to the base year simulation, including meteorology, photolysis rates, landuse, and other inputs. Thus, the only changes between the 2006 and 2010 CAMx modeling databases will be anthropogenic emissions and possibly BCs.

7.5 Emissions Sensitivity Experiments

Model sensitivity experiments are a vital and mandatory component of an 8-hour ozone SIP attainment demonstration analysis – both for the base case performance assessment (see Chapter 6) as well as in the future year control strategy assessment and uncertainty analysis.

Turning specifically to the future year assessments, sensitivity analyses are designed to facilitate the emissions control scenario identification and evaluation process. Today, four complimentary "Probing Tools" can be used in the CAMx regional photochemical model. These methods include: (a) traditional or "brute force" testing, (b) the direct decoupled method (DDM) sensitivity, (c) Ozone Source Apportionment Technology (OSAT), and (d) Process Analysis (PA). The Denver modeling team will use at least two types of emissions sensitivity testing methods with the CAMx 2010 future year simulations.

Traditional Sensitivity Testing: The modeling team will perform across-the-board emission reduction sensitivity runs on the 4 km grid for the July 5-30, 2006 period reducing anthropogenic VOC or NOx emissions (separately) by 20% from the 2010 base case conditions for the following source categories:

- On-road mobile sources;
- Non-road mobile sources;
- Oil and gas production sources;

- Other area sources; and
- Point sources.

In addition, we would perform an on-road mobile sources 20% co-emissions reduction sensitivity test. This results in eleven (11) 2010 emission reduction sensitivity tests. Two more additional 2010 sensitivity tests will be performed to be determined. These sensitivity runs serve two purposes, (a) they aid in helping to define more refined emissions control scenarios, and (b) they provide episode-specific model uncertainty information that may be used later in the "Weight of Evidence" analyses in support of the 8-hour ozone attainment demonstrations.

Ozone Source Apportionment: Ozone source apportionment will be used to obtain more refined ozone source-receptor relationships in the Denver region. The Anthropogenic Precursor Culpability Assessment (APCA) version of the Ozone Source Apportionment Technology (OSAT) will be used for 2010 base case emissions to: (a) assess the contribution of sources in the Colorado and surrounding states to ozone concentrations in key receptor areas in the Denver area, and (b) identify the particular source categories that may contribute the most to future-year elevated 8-hour ozone concentrations at various nonattainment monitors. Details on the CAMx ozone source apportionment are available in the CAMx User's Guide (ENVIRON, 2006; www.camx.com).

7.6 Control Strategy Development, Testing and Analysis

The general approach to be followed in assessing whether the Denver region is likely to be in attainment of the 8-hour ozone standard or whether and to what extent additional VOC and NOx emissions reductions will be required to achieve attainment will be consistent with the methodologies stipulated in EPA's recent 8-hour ozone modeling guidance (EPA, 2007). The procedure to be followed in performing the ozone attainment demonstrations is discussed in Chapter 8. The main theme of this approach is to use the model in a relative sense through model-derived site-specific relative response factors (RRFs) that are used to scale the current observed 8-hour ozone Design Values.

The CAMx 2010 future-year 8-hour ozone simulations will reveal the extent to which further emissions reductions are needed in the region to provide for attainment of the 8-hour ozone NAAQS by 2010. Should ozone violations be projected in the region in the future year simulation, the severity, location, and spatial extent of the modeled exceedances will be studied in order to postulate candidate emissions reductions strategies within and upwind of the nonattainment area. That is, should the future year modeling reveal a nonattainment problem, then an attainment demonstration analysis will be performed that will include the 8-hour ozone modeled attainment test, specific screening analysis and supplemental corroborative analyses set forth in the EPA guidance. These attainment demonstration procedures for ozone are described in detail in the following Chapter 8.

It is difficult when a modeling study protocol is first prepared to specify precisely the nature of the future year local and regional ozone control scenarios that may be required; indeed, the application of existing and mandated regional and local controls "on the books" and "on the way" (e.g., the effects of fleet turnover) could potentially and dramatically change the current attainment picture in the region. The RAQC and APCD will likely provide the modeling team with several alternative 2010 emission control strategies that will be modeled using the CAMx model and used to project 2010 8-hour ozone DVs for the Denver area following the procedures given in Section 8.

8.0 OZONE ATTAINMENT DEMONSTRATION

The ultimate objective of the Denver ozone modeling study is the development of modeling databases that can be used to define emissions control strategies that demonstrate future-year attainment of the 8-hour ozone National Ambient Air Quality Standard (NAAQS). This section describes the procedures for demonstrating future-year attainment of 8-hour ozone NAAQS.

8.1 Ozone Weight of Evidence Analyses

A central theme of EPA's 8-hour ozone modeling guidance document is the use of supporting corroborative analyses to bolster confidence that the selected control plan will in fact achieve attainment in the future-year (EPA, 2007). This corroborative analysis is part of the Weight of Evidence (WOE) used in a State Implementation Plan (SIP) to support the final control plan selection. Details of the WOE and types of corroborative analysis that can be used in an ozone attainment demonstration have been discussed earlier in Section1.5.8.

8.2 8-Hour Ozone Attainment Demonstration Procedures

The procedures for performing a modeled ozone attainment demonstration are outlined in EPA's 8-hour ozone modeling guidance (EPA, 2007). These procedures involve the use of the model in a relative sense to scale the observed site-specific 8-hour ozone Design Values (DVs) based on the relative changes in the modeled 8-hour ozone concentration between the current-year 2006 and 2010 future-year. The model-derived scaling factors are called Relative Response Factors (RRFs) and are based on the relative changes in the modeling results between the 2006 base case and the 2010 future-year emission scenarios.

The EPA guidance procedures for performing 8-hour ozone DV projections (EPA, 2007) have been codified in EPA's Modeled Attainment Test Software (MATS) tool. MATS includes ambient ozone air quality data and the user provides modeling results for the current year base case and the future year. MATS performs two types of 8-hour ozone DV projections: (a) projections at monitoring sites with observed 8-hour ozone Design Values; and (b) unmonitored area screening analysis 8-hour ozone projections that interpolates the observed 8-hour ozone DVs across the modeling domain to obtain gridded fields of 8-hour ozone DV projections.

The general procedures for projecting 8-hour ozone DVs at a monitoring site given in EPA's guidance are as follows (EPA, 2007):

- The starting point for the 8-hour ozone DV projections is the current year Design Value (DVC) that EPA guidance suggests should be based on the average of three 3-year periods of 8-hour ozone DVs centered on the modeling year. This results in a DVC that is a "5-year DV" that is used as the starting point for the 8-hour ozone DV projections. For the 2006 modeling year, this would mean averaging the 2004-2006, 2005-2007 and 2006-2008 8-hour ozone DVs at each ozone monitoring site in Denver. As data for 2008 are not yet available, we proposed at alternative approach to just use the standard 3-year DV from 2005-2007 as the starting point for the projections;

- Perform 2006 base year modeling on the 36/12/4 km grid for the June-July 2006 episode using the 2006 Typical base case emissions;
- Perform 2010 future-year base case and control strategy modeling on the 36/12/4 km grid for the June-July, 2006 meteorological conditions;
- Develop RRFs, defined as the ratio of the average of 8-hour daily maximum ozone concentrations "near" each monitor for the 2010 future year emission scenarios to the 2006 base year for all days in which the 2006 base case ozone values are above a "threshold" value:
    - Here, "near" the monitor is defined as a grid cell size dependent array of cells centered on a monitor, where EPA guidance suggest that the arrays be 1x1 for 36 km, 3x3 for 12 km and 7x7 for 4-km grid cells. However, given the complex terrain in the Denver region and close proximity of some of the monitoring sites, a 7x7 array of 4 km grid cells may be too large and not capture local-specific conditions of a monitor. Thus, we intend to examine the effects of using different array sizes for the purpose of performing 8-hour ozone DV projections and conduct sensitivity analysis of this parameter.
    - EPA's 8-hour ozone guidance specifies that RRFs should be calculated using all days with base-year ozone concentrations near the monitor greater or equal to 85 ppb, and also recommends that at least 10 modeling days should be included – these two recommendations may be in conflict:
        - In the event that there are less than 10 modeling days with base year daily maximum 8-hour ozone concentrations near the monitor $\geq$ 85 ppb threshold then:
            - The threshold is successively reduced by 1 ppb (e.g., 84 ppb, 83 ppb, etc.) until 10 modeling days are obtained; or
            - A 70 ppb threshold floor is imposed;
        - If there are still less than 10 days upon reaching the 70 ppb threshold then:
            - If there are 5 or more days, proceed with the attainment demonstration but the results should be analyzed carefully to be sure no single day is producing unusual model signals; or
            - If there are less than 5 days the issue will be discussed with RAQC, CDPHE/APCD and EPA;
- Apply the modeled-derived RRFs to the DVC at each ozone monitor to obtain a projected future year 8-hour ozone DV (DVF);
- Truncate the future-year DVF to the nearest ppb;
- Compare the projected 8-hour ozone at each monitor (DVF) with the 8-hour ozone standard, where if all projected 8-hour ozone values are 84 ppb or lower then attainment has been demonstrated;
- Even if the modeled future-year 8-hour ozone DVF is 85 ppb or higher, a WOE attainment demonstration may be possible using supportive, corroborative and additional analysis:

- In fact, EPA recommends that the WOE analysis be conducted with projected 8-hour ozone DVFs in the 82 to 87 ppb range;
- EPA notes that for projected 8-hour ozone DVFs of 88 ppb or higher no amount of supportive information would likely be convincing for an attainment demonstration.

8.3 Exceptions to EPA Guidance

There are two exceptions we are making to the recommended future-year 8-hour ozone DV projection procedures in the EPA guidance.

8.3.1 Current Year Design Value (DVC) Used in Projections

EPA guidance recommends using an average of three years of 8-hour ozone DVs centered on the modeling year as the current year Design Value (DVC) starting point for the future year 8-hour ozone projections ("5-year DV"). For the June-July 2006 modeling period this would include observed ozone from 2004-2008 period and since 2008 data have not yet been collected this is not possible. A possible alternative to this would be to use a "4-year DV" based on 2004-2007 data as the DVC starting place for the 8-hour ozone projections. However, this would include the relative clean years of 2004 and 2005 in the DVCs and in fact would result in all DVCs being below the 8-hour ozone NAAQS which would make the reliability of the 8-hour ozone projection procedure highly questionable. Thus, we propose to use the normal 3-year 8-hour ozone DVs from 2005-2007 as the DVCs, which is the period that determined whether the Denver area is an ozone nonattainment area or not.

Even with the DVCs based on the 2005-2007 3-year period, the Fort Collins West (FTCW) monitor would still not have any 8-hour ozone projections since data has only been collecting data for the 2006 and 2007 years. However, based on these two years of data the FTCW is the second most critical monitor, behind RFNO, so cannot be neglected. The modeling team will discuss this issue with RAQC, APCD and EPA and develop an appropriate DVC for FTCW so that 8-hour ozone projection sensitivity tests can be conducted for the FTCW monitor.

8.3.2 Definition of Near the Monitor

When 4 km grid spacing is used, EPA recommends that RRFs be based on the modeled highest daily maximum 8-hour ozone concentrations located within a 7x7 array of 4 km grid cells centered on the monitor. Given the complex flow conditions in the Denver, there are quite different characteristics between ozone monitors located in close proximity to each other and use of such a large array of cells could fail to capture some unique local characteristics of a specific monitor. For example, the RFNO and SBC monitors are located in fairly close proximity to each other yet record very different ozone levels and use of a 7x7 array of cells to define near the monitor would essentially result in using the same modeled ozone results in the RRFs for these two monitors failing to account for their individuality. Thus, we propose to perform array size sensitivity tests in the monitored 8-hour ozone projection sensitivity tests using arrays sizes of 1x1, 3x3, 5x5 and 7x7 around each monitor to define "near the monitor."

8.4 Unmonitored Areas Attainment Test

The MATS tool includes an unmonitored area attainment test to examine for potential 8-hour ozone hotspots away from the monitors. Given the uncertainties in these procedures, EPA guidance is clear that projected 8-hour ozone DVs exceeding the NAAQS away from the monitors do not necessarily imply that the NAAQS would be violated, rather they suggest an unmonitored location where high ozone could be occurring and additional ozone monitors should be deployed to determine whether the location is a potential trouble spot.

The MATS procedures for conducting the unmonitored area attainment test are as follows:

- Interpolate the DVCs from the monitoring sites to each grid cell in the modeling domain;
- Calculate gridded RRFs for each grid cell using the ratio of the average modeled future-year to current-year concentrations in each grid cell for all days in which the current-year daily maximum 8-hour ozone concentrations exceeds a threshold value (again a threshold of 85 ppb is used initially that is reduced until at least 10 days are included in the RRFs with a 70 ppb threshold floor); and
- The gridded RRFs are applied to the gridded DVCs to obtain an array of gridded future-year projected DVs (DVFs).

Note that it is likely that portions of the modeling domain will have no projected DVFs because there were insufficient ozone days above 70 ppb to construct an RRF.

For the Denver 2010 ozone modeling, we will perform the MATS unmonitored area attainment test using the 2005-2007 DVCs discussed previously.

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