

Development of the CAMx One-Atmosphere Air Quality Model to Treat Ozone, Particulate Matter, Visibility and Air Toxics and Application for State Implementation Plans (SIPs)

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ABSTRACT

The Comprehensive Air-quality Model with extensions (CAMx) is a photochemical grid model developed to treat urban and regional scale air quality issues using the one-atmosphere concept. Since its initial development in the late 1990s, the model has undergone continuous development and refinements. This paper presents the recent developments of the CAMx model including the extension to treat particulate matter (PM) and visibility, urban air toxics and mercury. Recent updates to the April 2003 release of the one-atmosphere CAMx versions 4 PM/ozone model are discussed along with the development of the full-science PMCAMx. The paper also discusses several current CAMx ozone modeling applications to support the development of 1-hour ozone and 8-hour ozone State Implementation Plans (SIPs) including several as part of the 8-hour ozone Early Action Compact (EAC) analysis.

INTRODUCTION

The Comprehensive Air-quality Model with Extensions (CAMx) is a three-dimensional multi-scale photochemical grid model¹ that is publicly available without fees or restrictions on model application (www.camx.com). CAMx was developed with all new code during the late 1990s using modern and modular coding practices. Initial applications focused on ozone impacts in the eastern United States as part of the Ozone Transport Assessment Group (OTAG).^{2,3,4} More recently it has been adopted as one of the primary ozone modeling platforms for ozone State Implementation Plan (SIP) modeling. CAMx has, or is, being used in 1-hour ozone SIP modeling for Houston⁵, Dallas Fort Worth⁶ and areas in California⁷, as well as 8-hour ozone Early Action Compact (EAC) SIP modeling for Denver⁸, Tulsa⁹, East Texas¹⁰, San Antonio¹¹, Austin¹¹ and San Juan County, New Mexico.¹² The modern and modular CAMx code has made the model an ideal platform for extension to treat a variety of air quality issues including ozone, particulate matter (PM)¹³, visibility, acid deposition and air toxics.¹⁴ The flexible CAMx framework has also made it a convenient and robust host model for the implementation of “probing tool” techniques such as Process Analysis, the Decoupled Direct Method (DDM) and the Ozone Source Apportionment Technology (OSAT).^{15,16,17}

CAMx Version 4

CAMx Version 4 (CAMx4)¹ was first released in April 2003 and includes a one-atmosphere treatment of ozone and particulate matter. CAMx Version 4 was the first update since CAMx Version 3.10 released in June 2002 and includes the following improvements:

- Two-section treatment of particulate matter (PM) that separately treats fine (<2.5 :) and coarse (2.5-10 :) PM that includes the following science algorithms:
 - ISORROPIA^{18,19} gas/particle partitioning aerosol thermodynamics module;
 - RADM²⁰ aqueous-phase chemistry module; and
 - SOAP²¹ Secondary Organic Aerosol (SOA) module.
- Updates to wet scavenging that separate treats in cloud rainout with below cloud washout and accounts for mass transfer of gaseous species as raindrops evaporate before they hit the ground.¹
- Addition of a Reactive Tracer (RTRAC) “probing tool” to simulate gaseous and particulate reactive tracers that operate in parallel to the host model extracting chemistry and deposition information that can be used to address:
 - Air toxics compounds whose results can be used with a near-source plume model to account for both the hot-spot fence-line impacts along with the regional background in a mass consistent fashion¹⁴;
 - Individual VOC compounds for verifying emission inventory speciation assumptions and better evaluation of the modeling system; and
 - Simulate source-receptor relationship of primary emitted contributions and contributions of primary versus secondary pollutants.
- Various other updates to improve the usability and technical formulation of the model.

Development of PMCAMx

In parallel to the development of the one-atmosphere CAMx4 model, ENVIRON, with Carnegie Mellon University (CMU) and Sonoma Technology, Inc. (STI), developed the full-science PMCAMx model by implementing the state-of-science PM modules developed by CMU into the CAMx V3.01 code. The full-science PMCAMx code includes the following science components:

- Size distribution is represented using the Multi-component Aerosol Dynamics Model (MADM), which uses a sectional approach to represent the aerosol particle size distribution.²² MADM treats the effects of condensation/evaporation, coagulation and nucleation upon the particle size distribution.
- Inorganic aerosol thermodynamics are represented using ISORROPIA^{18,19} within MADM.
- Secondary organic aerosol thermodynamics are represented using the semi-volatile scheme of Strader and co-workers.²¹
- Aqueous-phase chemical reactions are modeled using the Variable Size-Resolution Model (VRSM) of Fahey and Pandis²³, which automatically determine 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 CAMx deposition algorithms were improved for particle deposition. Dry deposition is represented for the size-resolved particle distribution.¹ A new wet deposition algorithm has also been developed, but was not implemented in the initial PMCAMx version 3.01.

The new PMCAMx model has been evaluated for a Los Angeles PM episode as well as for the Midwestern US.²⁴ These preliminary results suggest that the model exhibits some skill in predicting sulfate and nitrate and other PM components.

Current CAMx development activities include implementation of the PMCAMX full-science PM algorithms within CAMx4 so that the one-atmosphere and full-science PM algorithms are available within the same platform.

CURRENT REGULATORY APPLICATIONS OF THE CAMx MODEL

To address the regional haze rule, five Regional Planning Organizations (RPOs) were formed that consist of groups of states, tribes, federal agencies and stakeholders. These RPOs are testing and evaluating different regional PM models for use in developing regional haze plans that are due in 2007. The RPOs will also assist states in the development of their fine particulate plans that are also due in 2007. EPA's Models-3 Community Air Quality (CMAQ)²⁵ modeling system is the primary model being evaluated by the most of the RPOs for future-use in the regional haze and fine particulate SIPs, however the CAMx model is also being considered by some of the RPOs.

Although CAMx is one of the models being considered for the future 2007 regional haze and PM_{2.5} SIPs, current regulatory applications are focusing on 1-hour and 8-hour ozone attainment activities that are described next.

1-Hour Ozone SIP Modeling

Current (2003) 1-hour ozone SIP modeling activities are focusing on "mid-course correction" to evaluate and update, as necessary, 1-hour ozone attainment emission control plans developed in previous 1-hour ozone SIPs. Some example areas currently using CAMx for their 1-hour ozone SIP modeling include:

Dallas-Fort Worth: To support the Dallas-Fort Worth 1-hour ozone mid-course correction SIP an all new August 1999 episode is being modeled using the MM5 meteorological, EPS2x emissions and CAMx photochemical models.²⁶ Preliminary modeling mostly achieves EPA performance goals and is consistent with the 1-hour ozone SIP modeling.

Houston-Galveston: The current Houston-Galveston area (HGA) SIP is based on CAMx modeling of a September 1993 episode. In the year 2000 the TexAQS 2000 field study was conducted that emphasizes our understanding of 1-hour ozone exceedances in the HGA. High temporal resolution ozone and VOC measurements has revealed the presence of plumes of highly reactive VOCs that cause rapid rises in ozone concentrations. This finding has developed the concept of Transient High Ozone Events (THOES) that are defined as changes in ozone concentrations from one hour to the next of 60 ppb or greater. These findings refocus the HGA ozone attainment control plan to include controlling the release of these highly reactive VOCs, that are believed to come from chemical plants and refineries along the Galveston Bay and ship channel, along with the more traditional VOC/NOx control strategy. Currently the CAMx model

is being applied to an August-September TexAQS2000 episode using MM5 and RAMS meteorological to incorporate this new information into the HGA 1-hour ozone mid-course correction SIP.²⁷

San Francisco Bay Area: The CAMx model is being applied to central California for year 2000 Central California Ozone Study (CCOS) episodes to develop a 1-hour ozone control plan for the San Francisco Bay Area.⁷

8-Hour Ozone SIP Modeling

EPA currently plans to designate 8-hour ozone nonattainment areas in April 2004, in which case the first 8-hour ozone attainment SIPs are due in 2007. For areas that are currently attaining the 1-hour ozone standard, but may violate the 8-hour ozone standard, EPA has developed the concept of an 8-hour ozone Early Action Compact (EAC) in which local areas agree to implement emission controls early on, as necessary, and demonstrate that the 8-hour ozone standard will be achieved by 2007. In return, EPA will defer the designation of the region as being in nonattainment of the 8-hour ozone standard that is scheduled for April 2004 until 2007, as long as all the 8-hour EAC requirements are met. Key milestone dates in the 8-hour ozone EAC process are as follows:

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

CAMx is currently being used to develop emissions control plans for several 8-hour ozone EAC SIPs including:

Denver: CAMx is being applied for the 50 day period of June 7 through July 22, 2002 to address 8-hour ozone issues in Denver.⁸ This period contains three 8-hour ozone exceedance episodes in Denver: June 8-12, 2002; June 25 – July 1, 2002; and July 18-21, 2002. The model is being performed using a 36/12 km grid covering the western US for the entire 50 day period and using a 4/1.33 km grid during the episodes.

Oklahoma: The period of July 13 through August 1, 1999 is being simulated by CAMx to address 8-hour ozone issues in Oklahoma.⁹ During this period, 8-hour ozone exceedances occurred in both the Tulsa and Oklahoma City areas. Meteorological and emission inputs are being generated by the MM5 and EPS2x models, respectively.

San Juan County, New Mexico: CAMx is also being applied to the Four Corners areas for a June/July 2002 episode to support the development of an 8-hour ozone EAC plan for San Juan County, New Mexico.¹²

Texas Areas: The cities of Austin, Longview, San Antonio and Tyler are all developing 8-hour ozone EAC plans. Episodes from August and September 1999 are being simulated using the CAMx model with inputs developed by MM5 and EPS2x.¹¹

EMERGING ISSUES IN 8-HOUR OZONE MODELING

There are several emerging issues in 8-hour ozone modeling to support development of the 8-hour ozone SIPs that need to be addressed and refined. Currently there is only draft 8-hour ozone modeling guidance from EPA.²⁸ The draft guidance suggests new procedures for demonstrating attainment of the 8-hour ozone standard using Relative Reduction Factors (RRFs) and new model performance ozone metrics and performance goals related to 8-hour ozone. For traditional 8-hour nonattainment areas whose SIP's will be due in 2007 EPA has time to test and refine the draft 8-hour ozone modeling guidance. However, for those areas embarking on an 8-hour ozone EAC whose SIPs are due in 2004, the draft 8-hour modeling guidance is currently being applied. Thus, the draft guidance is being interpreted and the results being run by EPA for their applicability.

Draft 8-Hour Ozone Guidance Attainment Test

EPA's draft 8-hour ozone guidance recommends using the model in a relative sense to demonstrate attainment of the 8-hour ozone standard. That is, the ratio of the modeling results for the future year control strategy to the current year base case is used to scale the current year 8-hour ozone Design Value (DVC) to estimate the future year 8-hour ozone Design Value (DVF) that is compared against the 8-hour ozone standard to determine whether attainment has been demonstrated. This is done using a modeled Relative Reduction Factor (RRF) at each ozone monitor i:

$$DVF_i = RRF_i \times DVC_i$$

Where,

DVC_i is the current year 8-hour ozone Design Value at monitor i.

RRF_i is the relative reduction factor calculated "near" monitor that is the ratio of the future year 8-hour daily maximum concentration predicted "near" a monitor (averaged over several days) to the current year 8-hour ozone daily maximum concentrations predicted "near" the monitor (averaged over the same days).

DVF_i is the future year estimated 8-hour ozone Design Value at monitor i.

The EPA definition of "near" the ozone monitor depends on grid resolution. It is defined as an array of NX by NY grid cells centered on the monitoring location that completely encompasses a circle of radius 15 km from the monitor. For example, a 7 x 7 array of cells is used for a 5 km grid, 3 x 3 array for a 12 km grid, 1 x 1 array for a 36 km grid, etc. For the attainment test, the estimated maximum 8-hour ozone concentration within the array of cells near the monitor i is selected from the current year base case ($O3C_{ij}$) and future year control strategy ($O3F_{ij}$) for each modeling day j. The RRF is then obtained as the ratio of the future year control strategy to current year base case estimated average 8-hour ozone concentration near monitor i averaged over all days in which the base case 8-hour ozone value near the monitor is greater than 70 ppb.

$$RRF_i = \left[\sum_j O3F_{ij} \right] / \left[\sum_j O3C_{ij} \right]$$

Draft 8-Hour Ozone Performance Metrics and Goals

Table 1 summarizes several of EPA’s new ozone model performance tests from their draft 8-hour ozone modeling guidance.²⁸ One of the new ozone performance metrics listed in EPA’s draft 8-hour modeling guideline is as follows:

“bias pred/obs mean 8-hr (& 1-hr) daily maxima near each monitor”²⁸

The performance goal in EPA’s draft 8-hour ozone modeling guidelines for this ozone metrics is as follows:

“~20% most monitors (8-hr comparisons only)”²⁸

How “near each monitor” is defined and which estimated 8-hour ozone concentration to select “near” the monitor to compare with the observed 8-hour ozone concentration at the monitor is not defined in the draft guidance.

Elsewhere in the EPA draft 8-hour ozone modeling guidance under the attainment demonstration test using RRFs, EPA defines “near” as a block of NX by NY cells centered over the monitor that encompasses the circle with a radius of 15 km. When EPA was contacted they confirmed that this definition of “near” appeared to be a consistent and reasonable interpretation of the guidance when calculating the performance test also.

The next step in defining this 8-hour ozone performance metric was to determine which estimated daily maximum 8-hour ozone concentration should be selected from the array of NX by NY cells that defines “near” the monitor. We have developed three interpretations of the EPA guidance as follows:

- (1) Selection the maximum estimated daily maximum 8-hour ozone concentration “near” the monitor for comparison with the observed value. This interpretation is totally consistent with EPA’s draft 8-hour ozone guidance attainment test. However, it is an unbalanced approach that would tend toward an overestimation bias. Thus, care must be taken in the interpretation when comparing against EPA’s performance goal of within " 20% because an overestimation tendency may not necessarily indicate a poorly performing model. Thus, when using the maximum estimated daily maximum 8-hour ozone concentration “near” a monitor, only the less than –20% EPA performance goal should be used.
- (2) Selection of the best fit estimated daily maximum 8-hour ozone concentrations “near” the monitor. In this test the estimated 8-hour ozone concentrations within the NX by NY array of cells that matches the observed value most closely is selected for comparison. This test asks whether there is an estimated 8-hour ozone value near the monitor that matches the observed value. In this case, the within " 20% EPA performance goal is applicable.
- (3) The third approach uses the spatially paired value at the monitor. This is the most stringent definition of “near” the monitor as it spatially matches the prediction to the point location of the observation. Thus, the EPA within " 20% performance goal is not truly applicable.

When making the comparisons of predicted and observed daily maximum 8-hour ozone concentrations, a 60 ppb observed ozone cut off is used, as is used for 1-hour ozone performance comparisons.

Table 1. EPA’s draft 8-hour ozone modeling guidance ozone performance tests and goals.

Test(s)	Goals/Objectives	Comment
“bias pred/obs mean 8-hr (& 1-hr) daily maxima near each monitor” ¹	“~20% most monitors (8-hr comparisons only)” ¹	EPA’s draft modeling guidance does not define “near each monitor”. After discussing this issue with EPA “near” was defined to mean the same block of grid cells near the monitor used in EPA’s attachment test (e.g., 7 x 7 for 5 km grid). There are three ways we defined “near” for this metric: <ul style="list-style-type: none"> (1) Select the maximum predicted daily maximum 8-hr ozone concentrations “near” the monitor; (2) Select the predicted values closest in value to the observed value “near” the monitor; and (3) Select the predicted value at the monitor.
“Fraction bias pred/obs mean 8-hr (& 1-hr) daily maxima near each monitor” ¹	“~20% most monitors (8-hr comparisons only)” ¹	Define “near” the three ways described above.
“Correlation coefficients, all data, temporally paired means, spatially paired means” ¹	“Moderate to large positive correlations” ¹	Apply to three data sets described above.
“bias (8-hr daily max and 1-hr obs/pred), all monitors” ¹	“~5-15%” ¹	
“gross error (8-hr daily max and 1-hr obs/pred), all monitors” ¹	“~30-35%” ¹	
Partition data base into upwind, center city and downwind sites and repeat analysis		Get better ideas of level of model agreement based on upwind/downwind stratification and whether there is any obvious pattern of the model performance.
“Scatter plots & Q-Q plots of 8-hr and 1-hr metrics”		Applied to three sets of databases listed above.

¹ “Draft Guidance on the use of Models and other Analysis in Attainment Demonstrations of the 8-Hour Ozone NAAQS”²⁸

Example 8-Hour Ozone Performance Results

Using actual observed and preliminary modeled ozone results from a current 8-hour ozone Early Action Compact (EAC) study, examples of the three approaches above are used to demonstrate the new 8-hour ozone performance metric.

Figure 1 presents a scatter plot and a Q-Q plot of the predicted and observed daily maximum 8-hour ozone concentrations using the maximum predicted value “near” the ozone monitor. Of the 43 predicted/observed daily maximum 8-hour ozone concentrations above the 60 ppb observed ozone cut off, there are 6 points that are above the +20% performance goal and no points that are below the -20% performance goal. Thus, approximately 90% of the estimated daily maximum 8-hour ozone concentration maximums “near” the monitor across all monitors and modeling days achieve the within " 20% EPA performance goal. The 6 points above the +20% performance do not necessarily indicate a model performance problem when using the maximum estimated 8-hour ozone concentration near a monitor as such a condition could exist with a perfect model. The correlation coefficient is 0.51 and the Q-Q plots indicate the model estimated maximum 8-hour ozone concentrations near the monitor is reproducing the observed 8-hour ozone concentrations at the monitor with a slight overestimation tendency.

Figure 2 displays the predicted and observed 8-hour ozone comparisons using the best fit near the monitor ozone metric. In this case, all model/observation comparisons are within the " 20% performance goal and the Q-Q plots indicates that the best fit predicted and observed 8-hour ozone concentrations have the same frequency distribution. The correlation coefficient is high and close to 1 (0.94).

Figure 3 displays a comparison of the predicted and observed daily maximum 8-hour ozone concentrations spatially paired at the ozone monitor. Although not really applicable, it is useful to compare this more stringent test of the model against EPA’s performance goal. In this case there are 3 data points that exceed the " 20% performance goal so that approximately 95% of the monitoring site-days achieve the EPA performance goal. The Q-Q plot suggest an underestimation of the observed frequency below 100 ppb, but good agreement of the observed 8-hour ozone frequency distribution at higher levels of observed 8-hour ozone concentrations.

Thus, this example appears to be a situation in which the $\pm 20\%$ performance goal is being met.

Figure 1. Predicted and observed daily maximum 8-hour ozone concentrations using the maximum predicted value “near” the ozone monitor, open circles compare 5 percentiles of the predicted and observed frequency distribution of 8-hour ozone concentrations.

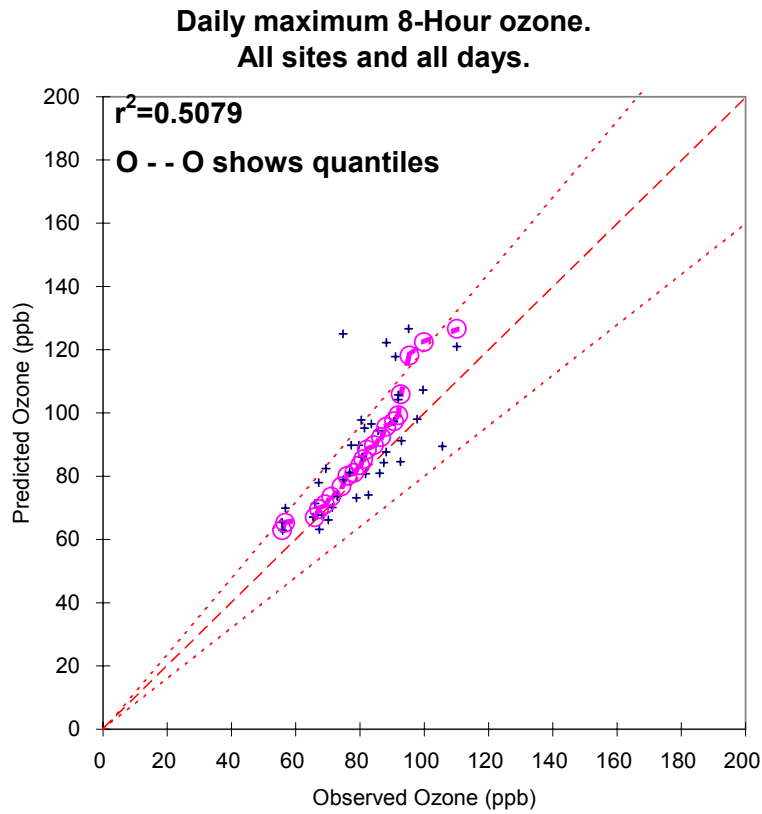


Figure 2. Predicted and observed daily maximum 8-hour ozone concentrations using the best fit predicted value “near” the ozone monitor, open circles compare 5 percentiles of the predicted and observed frequency distribution of 8-hour ozone concentrations.

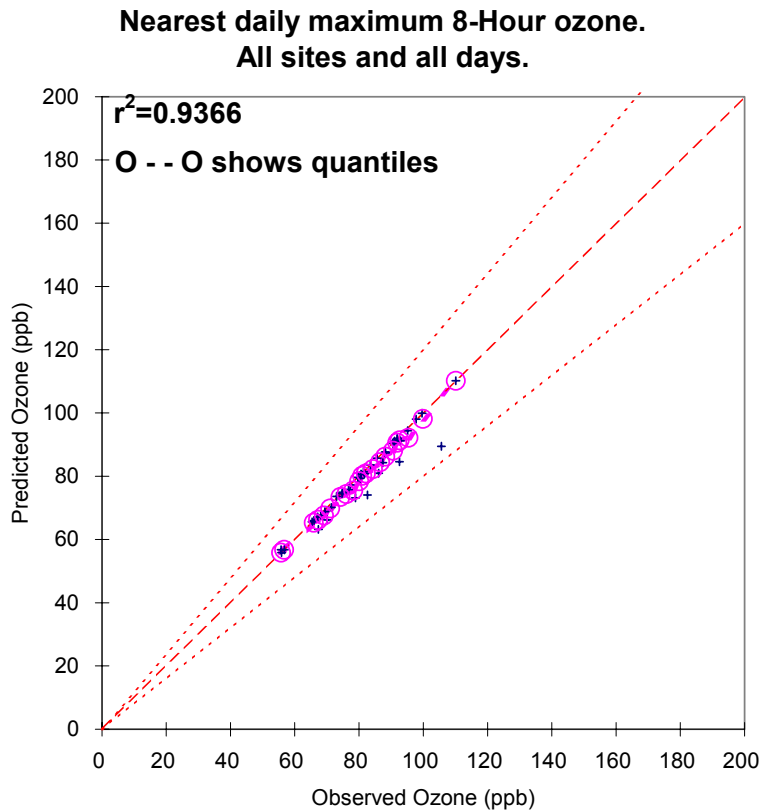
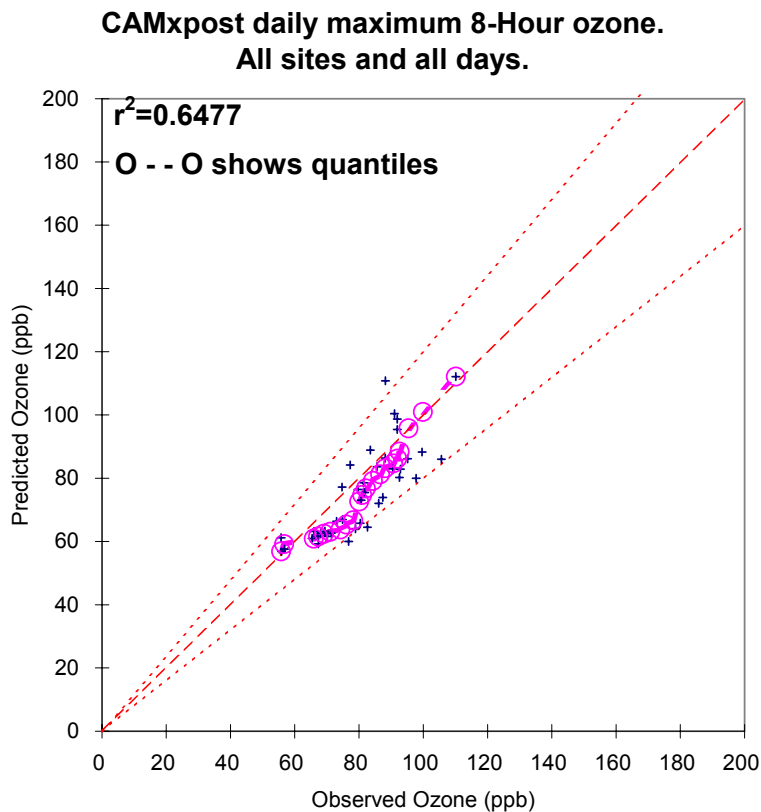


Figure 3. Predicted and observed daily maximum 8-hour ozone concentrations using the spatially paired predicted value at the ozone monitor, open circles compare 5 percentiles of the predicted and observed frequency distribution of 8-hour ozone concentrations.



CONCLUSIONS

The CAMx model is a current state-of-science photochemical grid model that has been extended to treat particulate matter (PM) and air toxics. It is flexible, computationally efficient and is being updated to possess both one-atmosphere ozone/PM science algorithms as well as full-science algorithms within the same platform. It is an ideal platform for addressing upcoming fine particulate (PM_{2.5}), regional haze issues and air toxics issues, as well as the current 1-hour and 8-hour ozone applications. One unique aspect of the CAMx model is the implementation of several probing tools that can be used to optimize control strategies and understand better source receptor relationships as well as the processes that govern ozone and PM formation. Currently implemented probing tools include the Ozone Source Apportionment Technology (OSAT), Decoupled Direct Method (DDM) and Process Analysis (PA), and work is ongoing to implement the PM Source Apportionment Technology (PSAT).

CAMx is currently being used to develop several 1-hour ozone Midcourse Correction State Implementation Plans (SIPs) as well as to develop several 8-hour ozone Early Action Compact (EAC) SIP control plans. These applications represent some of the first use of EPA's draft 8-hour ozone guidance. Preliminary 8-hour ozone EAC modeling results show how the draft EPA guidance performance goals can be used to assess whether the model is working sufficient well for demonstrating attainment of the 8-hour ozone standard.

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KEY WORDS

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