Diagnostic and Operational Evaluation of 2002 and 2005 Estimated 8-hr Ozone to Support Model Attainment Demonstrations

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1. INTRODUCTION

The United States Environmental Protection Agency (US EPA) promulgated nonattainment area designations for the 8-hour ozone National Ambient Air Quality Standard on April 15, 2004 (69 CFR 23858, April 30, 2004). State Implementation Plans will include modeling the impacts of emission control scenarios with 3-D Eulerian photochemical transport models. Several photochemical models, including the Comprehensive Air Quality Model with Extensions (CAMx4), treat the physical processes and chemistry that form ozone. Model performance is typically evaluated on an operational basis and rarely to support a diagnostic assessment. Operational evaluations for ozone modeling purposes include matching model estimates with observation data for ozone, nitrogen oxides (NO_X), and total volatile organic compounds (VOC).

A diagnostic evaluation assesses how appropriately the modeling system responds to emissions adjustments. Since the modeled attainment demonstration includes modeling current and future year emissions it is important to have confidence that the model will predict ozone concentrations appropriately when emissions change (US EPA, 2007). This type of evaluation includes modeling two different ozone episodes that are separated by enough years that large emissions differences exist. The diagnostic evaluation is an important assessment to make in addition to an operational evaluation because it is directly linked to the end use of the model, which is modeling the change in ozone concentrations after emissions adjustments.

A comparison between observed and estimated ozone for the summers of 2002 and 2005 is useful for a diagnostic assessment because high quality emission inventories were developed for each year and a large NO_X emissions reduction occurred between these years due in part to NO_X SIP Call compliance.

Modeling two full summer seasons provides an opportunity to make another diagnostic evaluation which assesses model performance for high ozone by day of the week. Emissions change substantially from weekday to weekend and having two full summers provides enough days with high ozone on each day of the week to make this type of evaluation useful.

A comparison of a typical summer day emission inventory used for this modeling application for the 5 State Midwest region (IL, IN, OH, MI, WI) is shown in Table 1.

Table 1. Typical July weekday emissions (tpd) for 2002 and 2005.

	VOC 2002	VOC 2005	NOX 2002	NOX 2005
Nonroad Mobile	1,167	1,558	1,875	1,843
Other Area	2,555	2,637	255	283
Onroad Mobile	2,185	1,829	4,035	3,402
EGU Point	35	28	3,422	1,712
Non-EGU Point	751	635	1,085	1,021
5 State Total	6,693	6,687	10,672	8,260

NO_X emissions over the Upper Midwest 5 State region decrease from 10,672 tpd to 8,260 tpd between 2002 and 2005. Most of this difference is attributable to a 1,710 tpd decrease in emissions from electrical generating utilities (EGUs) and a 633 tpd decrease in onroad motor vehicle emissions. Total VOC emissions are very similar between 2002 and 2005 for these 5 States. Emissions change between weekday and weekend in terms of total mass for VOC and NO_X, but they change in different directions which makes the mix of pre-cursors available on weekends different from weekdays. VOC emissions generally increase about 20% from weekday to

weekend due in large part to increases in off-road mobile source emissions. NO_X emissions decrease by 20% largely due to decreases in on-road mobile source and some decreases in electrical generating utility emissions.

The Midwest region experienced meteorology that is generally conducive for ozone formation in the summer of 2002 and 2005. A Classification and Regression Tree (CART) analysis was done examining meteorological data at certain locations in the Midwest United States to characterize how ozone conducive the summers of 2002 and 2005 were compared to other recent summers. CART is a non-parametric method that is advantageous because it is insensitive to distributions of variables, which means it is insensitive to missing data and outliers. CART classifies days into groups (or bins) based on meteorological characteristics associated with observed ozone from 1990 to 2006. The index is estimated based on the number of days in high ozone groups each year compared to the average number of days in those groups. A higher index value means the summer was more conducive to ozone formation. A zero value indicates that the summer was average in terms of meteorological characteristics conducive to ozone formation.

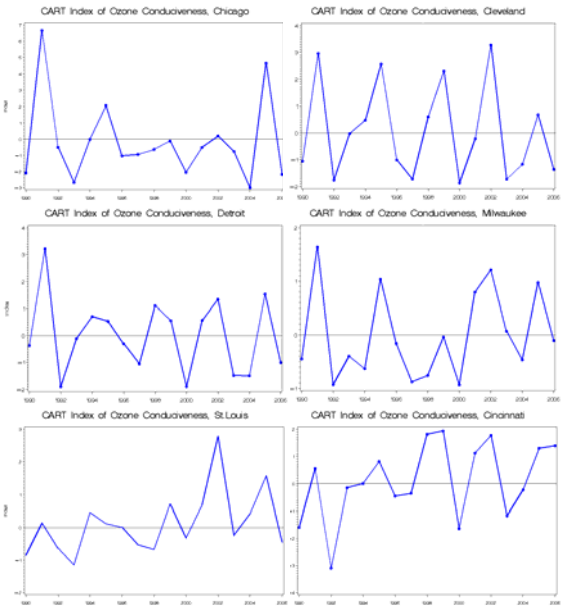

Fig. 1. CART ozone conducive index.

Figure 1 shows the estimated ozone conducive index from 1990 to 2006 at several locations: Chicago, Milwaukee, Cleveland, Cincinnati, Detroit, and St. Louis. At each of these locations the summers of 2002 and 2005 are at least typical in terms of ozone conduciveness and often have meteorological characteristics that are more conducive to ozone formation than a typical summer. This increases confidence that model estimates will largely be a response to differences in emissions rather than meteorology.

2. METHODS

The Comprehensive Air Quality Model with Extensions (CAMx) version 4.30 uses state of the science routines to model ozone formation and removal processes over regional and urban scales (Nobel et al, 2002; Chen et al, 2003; Morris et al, 2005). The model is applied with an updated carbon-bond IV (CB4) gas phase chemistry module (ENVIRON, 2006; Carter, 1996). CAMx is applied using the PPM horizontal transport scheme and an implicit vertical transport scheme with the fast CMC chemistry solver (ENVIRON, 2006). The photochemical model is initiated at midnight Eastern Standard Time and run for 24 hours for each episode day. The summer simulations are initiated on June 2 and run through August 31. The first 11 days of the simulation are not used in any analysis to minimize the influence of initial concentrations (Baker, 2007).

Boundary conditions represent pollution inflow into the model from the lateral edges of the grid and initial conditions provide an estimation of pollution that already exists. The initial and boundary conditions are based on monthly averaged species output from an annual (calendar year 2002) application of the GEOS-CHEM global chemical transport model (Jacob et al, 2002; Bey et al, 2001). Boundary conditions vary by month and in the horizontal and vertical direction. Where an initial or boundary concentration is not specified for a pollutant the model will default to a near-zero concentration.

The meteorological, emissions, and photochemical models are applied with a

Lambert projection centered at (-97, 40) and true latitudes at 33 and 45. The 36 km photochemical modeling domain consists of 97 cells in the X direction and 90 cells in the Y direction covering the central and eastern United States (Figure 2). The 2-way nested 12 km domain covers most of the upper Midwest region with 131 cells in the X and Y directions. CAMx is applied with the vertical atmosphere resolved with 16 layers up to approximately 15 kilometers above ground level.

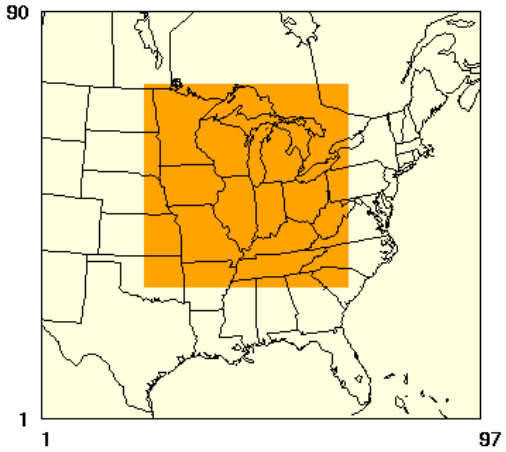

Fig. 2. 36 km (large box) and 12 km (small dark box) modeling domain.

Meteorological input data for the photochemical modeling runs are processed using the National Center for Atmospheric Research (NCAR) 5th generation Mesoscale Model (MM5) version 3.6.1 (Dudhia, 1993; Grell et al, 1994). Important MM5 parameterizations and physics options include mixed phase (Reisner 1) microphysics, Kain-Fritsch 2 cumulus scheme, Rapid Radiative Transfer Model, Pleim-Chang planetary boundary layer (PBL), and the Pleim-Xiu land surface module. Analysis nudging for temperature and moisture is only applied above the boundary layer. Analysis nudging of the wind field is applied above and below the boundary layer. These parameters and options are selected as an optimal configuration for the central United States based on multiple MM5 simulations using a variety of physics and configuration options (Johnson, 2003; Baker, 2004).

Emissions data is processed using EMS-2003. In addition to extensive quality assurance and control capabilities, EMS-2003 performs basic emissions processes such as chemical speciation, spatial allocation, and temporal allocation (Janssen and Hua, 2007; Wilkinson et al, 1994). Anthropogenic emission estimates are made for a weekday, Saturday, and Sunday for each month. The biogenic emissions are day-specific. Volatile organic compounds are speciated to the Carbon Bond IV (CB4) chemical speciation profile (Gery et al, 1989). Biogenic emissions are estimated with EMS-2003 using a variation of the BEIS3 model (Guenther et al, 2000). The BELD3 land use dataset is input to the biogenic model for fractional land-use and vegetative speciation information (US EPA, 2006; Kinnee et al, 1997). Other inputs to the biogenic emissions model include hourly satellite photosynthetically activated radiation (PAR) and 15 m (above ground level) temperature data output from MM5 (Pinker and Laszlo, 1992).

3. RESULTS & DISCUSSION

The ozone design value is the 4th highest maximum 8-hr ozone concentration over a summer averaged over 3 consecutive summers. The 95th percentile ozone concentration over each summer of 2002 and 2005 was chosen as a value similar to averaging 3 consecutive 98th percentile values together. The 95th percentile daily maximum 8-hr ozone observation for each monitor over each summer is paired with model estimates. The mean bias of 8-hr maximum ozone greater than the 95th percentile averaged over all stations in the 12 km domain is -13 ppb for 2002 (N=1,385) and -9 ppb for 2005 (N=1,677). The mean error of 95th percentile 8-hr maximum ozone is 15 ppb for 2002 and 12 ppb for 2005. NO_X and total VOC are only measured at a few sites in the region. In general, the modeling system shows little bias in estimating NO_X and total VOC in 2002 and has a slight over-estimation tendency of VOC in 2005.

The correlation coefficient is estimated to determine the relationship between the change in 95th percentile observations between 2002 and 2005 and the change in the paired model predictions between the

same years. This approach is designed to determine if the change in high ozone observed at each monitor location between 2002 and 2005 is similar to the change in model estimates of high ozone between 2002 and 2005 at the same location. If observed ozone decreases but the modeling system predicts similar values or an increase between years then the relationship would be weak. However, if the model predictions change similarly to the observed values then the relationship would be strong. The relationship in bias between 2005 and 2002 observations and the bias between paired predictions is strong (r=.64, r^2=.41, N=240). This indicates that the modeling system generally replicates the direction ozone observations are changing between 2002 and 2005 at upper Midwest monitor locations.

Another way to assess model response to emissions changes is to examine how well the model estimates high ozone by day of the week. Mean bias and mean error of days in each summer with 8-hr ozone greater than 80 ppb is shown in Table 2.

Table 2. Mean bias and mean error of days with 8-hr ozone > 80 ppb in 2002 and 2005.

Day of Week	N	Bias	Error
Monday	16	-11.8	18.1
Tuesday	14	-12.4	15.4
Wednesday	17	-15.5	18.2
Thursday	16	-13.8	17.4
Friday	17	-16.1	19.4
Saturday	14	-7.6	17.4
Sunday	16	-11.6	16.0

The benefit of simulating 2 summer seasons is that there are enough days with high ozone to assess model performance by day of the week. The results in Table 2 show consistent model performance by day of the week. The weekend days clearly do not perform any worse than weekday days. Again, the model seems to be responding appropriately to changes in the emission inventory.

4. CONCLUSION

The operational evaluation suggests high ozone is slightly under-predicted in both summers. The diagnostic approaches used in this study suggests the modeling system will appropriately respond to emissions adjustments, which is important since a relative modeling approach is required to estimate future year ozone values for ozone attainment demonstrations. Many different approaches may provide information useful to assess how appropriately the modeling system responds to emissions adjustments. Future research should explore other methods of diagnostic evaluation. One alternative approach involves modeling 2002 and 2005 anthropogenic emissions using 2002 meteorology and using the relative reduction factor approached detailed in the US EPA modeling guidance document to project 2005 values. These projected 2005 values could then be compared to observed values.

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