# OPERATIONAL AND DIAGNOSTIC EVALUATIONS OF THE OZONE FORECASTS BY THE ETA-CMAQ MODEL SUITE DURING THE 2002 NEW ENGLAND AIR QUALITY STUDY (NEAQS)

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## 1. INTRODUCTION

Ozone ($O_3$), a secondary pollutant, is created in part by emissions from anthropogenic and biogenic sources. It is necessary for local air quality agencies to accurately forecast ozone concentrations to warn the public of unhealthy air and to encourage people to voluntarily reduce emissions-producing activities.

## 2.0 DESCRIPTION OF THE ETA-CMAQ FORECAST MODEL SUITE AND OBSERVATIONAL DATABASE

The Eta-CMAQ air quality forecasting system is based on the National Centers for Environmental Prediction's (NCEP's) Eta model (Rogers et al., 1996) and the U.S. EPA's CMAQ Modeling System (Byun and Ching 1999). In this study, the modeling system is deployed over the domain of the northeast U.S. (Figure 1). The horizontal domain has a grid spacing of 12 km. 22 layers of variable thickness set on a sigma-type coordinate are used to resolve the vertical extent from the surface to 100 hPa. The primary Eta-CMAQ model forecast for next-day's surface-layer $O_3$ is based on the current day's 12 UTC Eta cycle. The target forecast period is local midnight through local midnight (04 UTC to 03 UTC for the Northeast U.S.).

The hourly $O_3$ data at 342 sites in the northeast U.S. are available from the U.S. EPA's AQS network (Figure 1). The four Atmospheric Investigation, Regional Modeling, Analysis, and Prediction (AIRMAP) sites and Harvard Forest (HF) provided continuous measurements of $O_3$ and related photochemical species as well as meteorological parameters during the NEAQS 2002 (see Figure 1). The four AIRMAP sites include Castle Springs (CS), Isle of Schoals (IS), Mount Washington Observatory (MWO), and Thompson Farm (TF) sites. $O_3$ Lidar vertical profiles obtained on the NOAA ship Ronald H. Brown during the NEAQS 2002 were used to assess the vertical concentrations. The model performance from August 6 to August 17, 2002, based on the 12 UTC run for the target forecast period is examined in this study.

## 3.0 RESULTS AND DISCUSSIONS

### *3.1 Operational evaluation over the NE U.S. domain at the AQS sites*

For the discrete evaluation, we calculated summary and regression statistics along with two measures of bias: the Mean Bias (MB) and the Normalized Mean Bias (NMB); and two measures of error: the Root Mean Square Error (RMSE) and Normalized Mean Error (NME) (see Table 1). The model reproduced 53.3, 88.6 and 83.5% of the observed hourly, maximum 1-hr and maximum 8-hr $O_3$ within a factor of 1.5, respectively. The recommended performance criteria for $O_3$ by U.S. EPA (1991) are: mean normalized bias ±5 to ±15%; mean normalized gross error 30% to 35%; unpaired peak prediction accuracy: ±15 to ±20%.

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The NMB and NME values for maximum 1-hr (maximum 8-hr) $O_3$ are 3.2% (9.0%) and 20.0% (21.8%), respectively, close to the performance criteria for the unpaired peak $O_3$.

For the categorical evaluation, we calculated model Accuracy (A), Bias (B), Probability Of Detection (POD), False Alarm Rates (FAR) and Critical Success Index (CSI) based upon observed (exceedances, non-exceedances) versus forecasted (exceedance, non-exceedances) for both the maximum 1-hr and 8-hr standard (Table 1). The Accuracy of the model prediction, which indicates the percent of forecasts that correctly predict an exceedance or non-exceedance, is very high (97.9%). However, the CSI value, which provides a measure of how well the exceedances were predicted, are 11.7% and 35.8% for the maximum 1-hr and 8-hr exceedances, respectively, indicating poor performance on reproducing the observed exceedances.

### *3.2 Diagnostic evaluation during the 2002 NEAQS*

Figure 2 presents an example of time-series comparisons and scatter plots of the model predictions and observations for $O_3$, NO, $NO_2$, CO, $NO_y$, and PAN at the HF site. The model captured the hourly variations and broad synoptic-scale changes seen in the observations of different gas species ($O_3$, $NO_2$, CO, $NO_y$, PAN, $SO_2$) (correlation coefficient>0.50, see Table 2) except NO at each site, although there were occasional major excursions. For the photolysis rates of $NO_2$, we focus our analysis on daytime data by excluding data where $JNO_2 < 5\times10^{-5}$ $s^{-1}$. Table 2 indicates that the model reproduced 77.1%, 64% and 70.9% of observed $JNO_2$ values within a factor of 1.5 at the CS, MWO and TF sites, respectively. DeMore et al. (1997) suggest that a ±20% uncertainty was associated with uncertainty in the cross-section and quantum yield data in the calculation of $JNO_2$ values. The sensitivity tests of Hanna et al. (2001) indicate that a 50% uncertainty in $NO_2$ photolysis rate could cause about a 40 ppbv, or a 20% uncertainty in predicted maximum $O_3$ concentration in their cases. This suggests that priority should be given to more accurate determination of the $JNO_2$ values in the model to get good $O_3$ predictions, especially during the cloudy periods as cloud cover can significantly affect the $JNO_2$ values.

Comparisons of modeled and ship-based Lidar observed $O_3$ vertical profiles provide an assessment for the ability of the model to simulate the vertical structure of air pollutants. Figure 3 indicates that while the model reproduced the observed vertical structure, it tended to overpredict in the higher layers.

The $[O_3]/[NOx]$ values can be used to determine $NO_x$-sensitive and VOC-sensitive chemical regimes. Following Arnold et al. (2003), the total hours spent in each extreme region and nearer to the $[O_3]$ ridgeline according to the $[O_3]/[NOx]$ values are calculated and listed in Table 3 for the HF, CS and TF sites. $[O_3]/[NOx]$ values >46 indicate strong $NO_x$-sensitive conditions, whereas its values <14 indicate VOC-sensitive conditions (Arnold et al., 2003). Table 3 reveals that for the most part, the model correctly reproduced the temporal variations in the observed $[O_3]/[NOx]$ ratios across the different conditions represented at the three sites.

The fraction of $NO_y$ converted to $NO_z$ can be used to represent the air mass photochemical age. It is found that the percentages of the daytime (6:00 to 18:00 EST) hours with air mass photochemical age values $[NO_z]/[NOy]$ >0.6 for the model are 96%, 56% and 87% at the CS, TF and HF sites, respectively, in agreement with the observations of 82%, 72% and 82% at the CS, TF and HF sites, respectively. These results are similar to those reported by Olszyna et al. (1994).

The $O_3$-CO correlations have been used to diagnose pollution influence of anthropogenic sources on $O_3$. Following Chin et al. (1994), we only used the observed data with $NO_x/NO_y<0.3$ (photochemically aged rural air) and obtained during the period from 13:00 to 17:00 LST. Strong correlations between $O_3$ and CO for both model predictions and observations with a consistent slope $?O_3/?CO$ indicate that the modeled lower limits of the ozone production efficiencies ($?_N$) values are close to the observations at the AIRMAP and HF sites. The upper limits of $?_N$ value can be estimated by the $O_3$-$NO_z$ slope. Following Arnold et al. (2003), both modeled and observed $O_3$-$NO_z$ slopes are obtained for only observational data with $[O_3]/[NOx]>46$ at the three sites. There is significant correlation between $O_3$ and $NO_z$ for both model predictions and observations ($r>0.77$) at the three sites (see Fig. 4). Both modeled and observed $?_N$ values at the three sites are in the estimated ranges (5 to 10) of other investigators (Olszyna et al., 1994) at rural sites in the eastern US, although the modeled $?_N$ values (4.3 to 5.1) are about half of the observations (8.3 to 10.0). The scatter plots of Figure 4 also show that the modeled $NO_z$ concentrations were higher than the observations, indicating that the model chemistry put more $NO_x$

into terminal products ($NO_y$) as opposed to $O_3$ than in real world.

## 4.0 REFERENCES


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Table 1. Operational evaluation on the basis of the AQS data over the northeastern US

| Discrete Statistics | | | | | |
|---|---|---|---|---|---|
| | RMSE (ppb) | MB (ppb) | NMB (%) | NME (%) | R |
| Hourly | 24.23 | 12.55 | 29.77 | 46.87 | 0.63 |
| Max 1-hr | 17.65 | 2.32 | 3.24 | 20.05 | 0.70 |
| Max 8-hr | 17.03 | 5.74 | 9.02 | 21.86 | 0.70 |
| Categorical Statistics | | | | | |
| | A (%) | B | FAR (%) | CSI (%) | POD (%) |
| Max 1-hr | 97.94 | 0.36 | 60.7 | 11.7 | 14.3 |
| Max 8-hr | 82.60 | 0.76 | 39.0 | 35.8 | 46.38 |

Table 2. Statistical summaries of the comparisons of the model results with the observations at the different sites during the 2002 NEAQS.

| | <C>* | | | | |
|---|---|---|---|---|---|
| Parameters | Obs | Model | r | % within a factor of 1.5** | % within a factor of 2** |
| **Castle Springs (N=288)** | | | | | |
| $O_3$ | 42.94 | 55.21 | 0.695 | 58.7 | 86.5 |
| NO | 0.15 | 0.03 | 0.172 | 9.3 | 18.1 |
| CO | 166.31 | 137.96 | 0.724 | 86.5 | 99.0 |
| $NO_Y$ | 2.91 | 4.15 | 0.800 | 46.5 | 76.7 |
| $SO_2$ | 1.29 | 2.46 | 0.751 | 23.4 | 44.7 |
| $JNO_2$ (1/S) | $4.37\times10^{-3}$ | $4.40\times10^{-3}$ | 0.971 | 77.1 | 91.4 |
| Temperature (C) | 24.61 | 23.59 | 0.962 | 99.0 | 100.0 |
| RH (%) | 53.22 | 51.23 | 0.843 | 98.6 | 100.0 |
| Wind direction | 221 | 264 | 0.212 | 76.7 | 85.1 |
| Wind speed (m/s) | 1.89 | 3.11 | 0.405 | 39.5 | 62.3 |
| **Harvard forest (N=288)** | | | | | |
| $O_3$ | 60.01 | 60.26 | 0.773 | 80.8 | 92.0 |
| NO | 0.16 | 0.09 | 0.467 | 36.8 | 55.6 |
| $NO_2$ | 1.85 | 1.97 | 0.443 | 38.4 | 60.5 |
| CO | 197.75 | 220.55 | 0.804 | 87.8 | 98.0 |
| $NO_Y$ | 6.10 | 9.20 | 0.766 | 40.1 | 74.1 |
| PAN | 0.62 | 1.23 | 0.690 | 24.2 | 47.2 |
| RH (%) | 74.08 | 60.65 | 0.882 | 96.6 | 100.0 |
| Wind direction | 242 | 261 | 0.002 | 88.9 | 90.5 |
| Wind speed (m/s) | 1.82 | 2.63 | 0.590 | 45.8 | 67.2 |
| **Isle of Schoals (N=288)** | | | | | |
| $O_3$ | 56.33 | 69.00 | 0.733 | 65.3 | 86.1 |
| CO | 237.93 | 168.00 | 0.631 | 48.1 | 90.6 |
| **Mount Washington (N=288)** | | | | | |
| $O_3$ | 60.65 | 53.11 | 0.827 | 86.3 | 99.3 |
| NO | 0.24 | 0.02 | 0.066 | 12.4 | 23.2 |
| CO | 154.59 | 119.68 | 0.639 | 82.7 | 96.0 |
| $SO_2$ | 1.23 | 1.52 | 0.662 | 33.2 | 48.4 |
| $JNO_2$ (1/s) | $4.01\times10^{-3}$ | $4.72\times10^{-3}$ | 0.917 | 64.0 | 77.7 |
| **Thompson Farm (N=288)** | | | | | |
| $O_3$ | 44.39 | 56.74 | 0.819 | 59.0 | 76.0 |
| NO | 0.16 | 0.19 | 0.636 | 23.7 | 42.0 |
| CO | 203.46 | 194.24 | 0.550 | 80.5 | 92.7 |
| $NO_Y$ | 4.60 | 9.51 | 0.505 | 25.1 | 51.6 |
| $SO_2$ | 1.94 | 7.64 | 0.028 | 13.8 | 18.5 |
| $JNO_2$ (1/s) | $4.32\times10^{-3}$ | $4.24\times10^{-3}$ | 0.944 | 70.9 | 86.3 |
| Temperature (C) | 24.09 | 24.40 | 0.942 | 100.0 | 100.0 |
| RH (%) | 64.26 | 55.38 | 0.834 | 92.0 | 100.0 |
| Wind direction | 231.07 | 229.13 | 0.452 | 87.2 | 95.5 |
| Wind speed (m/s) | 2.26 | 2.31 | 0.380 | 48.5 | 70.6 |

* <C> is the mean concentration (ppb)

** Percentages (%): are the percentages of the comparison points at which model results are within a factor of 1.5 and 2 of the observations. N is number of samples.

Table 3. Statistical summary of number of hours for response surface indicator ratios ($O_3/NO_x$) for model and observations at each sites during the period of August 6 to 17, 2002. The values in parentheses are the percentages (%).

| | Harvard Forest | | Castle Springs | | Thompson Farm | |
|---|---|---|---|---|---|---|
| $O_3/NO_x$ | Obs | Model | Obs | Model | Obs | Model |
| 0-14 | 28 (21) | 16 (12) | 1 (1) | 0 (0) | 16 (13) | 25 (21) |
| 15-25 | 11 (8) | 26 (20) | 13 (11) | 0 (0) | 13 (11) | 10 (8) |
| 26-45 | 11 (8) | 20 (15) | 12 (11) | 11 (10) | 16 (13) | 15 (13) |
| >46 | 83 (62) | 71 (53) | 88 (77) | 103 (90) | 75 (63) | 70 (58) |
| Total hours | 133 (100) | 133 (100) | 114 (100) | 114 (100) | 120 (100) | 120 (100) |

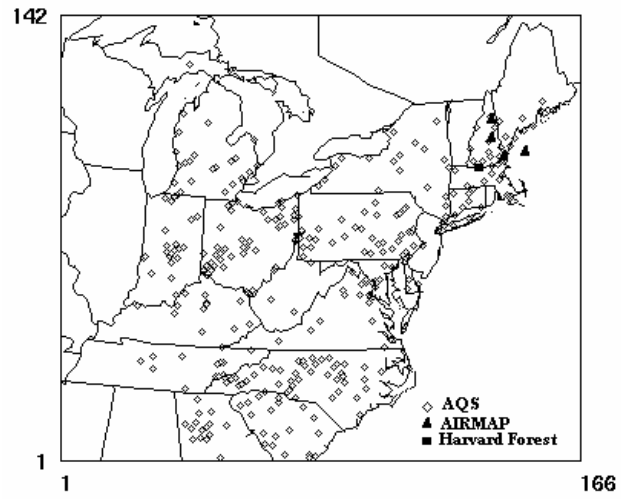


Fig. 1 The Eta-CMAQ model domain and locations of AQS, AIRMAP and Harvard Forest sites

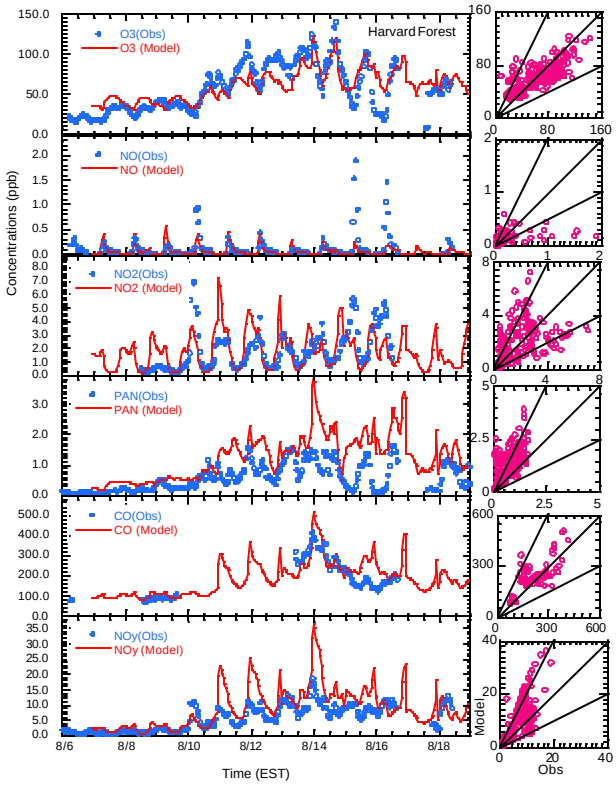


Fig. 2 Time-series and scatter plots of model predictions and observations at the Harvard Forest site

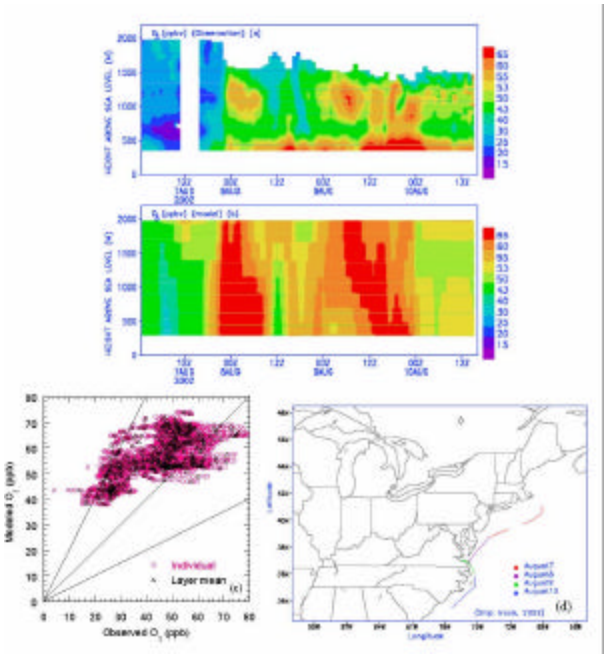


Fig. 3 Vertical $O_3$ profiles for the Lidar observations (a) and models (b) during the period from August 7 to 10, 2002. (c) scatter plots between the observations and model predictions for individual value and model-layer means and (d) ship tracks.

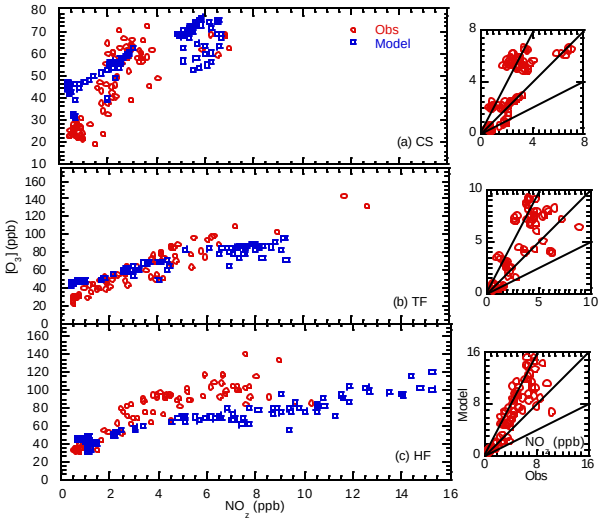


Fig. 4 $O_3$ as a function of $NO_z$ for the $NO_x$-limited conditions indicated by the observational data with $[O_3]/[NO_x]>46$ at (a) CS, (b) TF, and (c) HF. Right panels are scatter plots of modeled and observed $NO_z$.

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