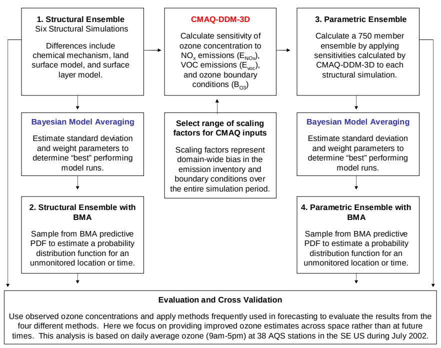
Probabilistic Estimates of Ozone Concentrations from an Ensemble of CMAQ Simulations

Kristen M. Foley[1], Robert W. Pinder[1], Sergey L. Napelenok[1], H. Christopher Frey[2]
1. USEPA Office of Research and Development, 2. North Carolina State University

INTRODUCTION

An ensemble of deterministic simulations is frequently used to create probabilistic estimates that account for uncertainty. A challenge with applying these approaches for simulations of ozone concentrations is that chemical transport models require significant input data and computational resources to complete a single simulation. This research offers a computationally efficient approach to create an ensemble using multiple configurations of the CMAQ air quality model and quantitative estimates of the uncertainty in three of the model inputs. A statistical method, known as Bayesian Model Averaging, is then used to post-process the ensemble of model runs based on observed ozone concentrations.

METHODS



CMAQ-DDM-3D

The Higher-Order Decoupled Direct Method in three dimensions is implemented in CMAQ version 4.5 (CMAQ-DDM-3D) for CB-IV and SAPRC99 chemical mechanisms. CMAQ-DDM-3D is used to estimate a reduced form model of ozone concentration to calculate the change in ozone as a result of increases/decreases in NO_x emissions (ENO_x), VOC emissions (EVOC), and ozone boundary conditions (BO3). Previous work has shown these to be among the inputs that have the most significant impact on ozone concentration. The model inputs are varied over a range based on previous studies and available data for this domain. The final result is a 750 member ensemble of ozone predictions for every grid cell and every day which reflects the uncertainty in the model form and input values.

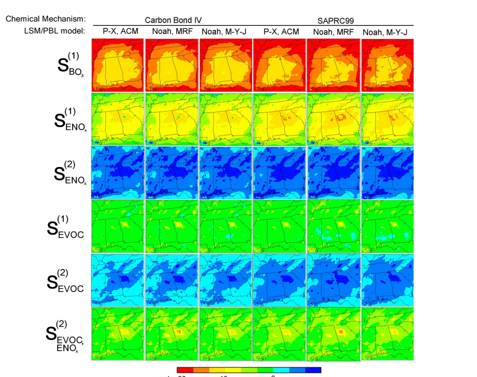


Figure 1. The first-order ($\mathbf{S}_j^{(1)}$), second-order ($\mathbf{S}_j^{(2)}$), and cross-sensitivity ($\mathbf{S}_{jk}^{(2)}$) of the ozone concentration to ozone boundary concentrations (BO_3), NOx emissions (ENO_x), and VOC emissions (EVOC) for each of the six structural uncertainty cases, averaged over the entire simulation period.

Bayesian Model Averaging

The BMA predictive PDF model for the ozone concentration at one location, *s*, and time, *t*, *y*(s,t), is expressed as a weighted average of normal distributions with means equal to the *K* different ensemble member predictions at that site and time, $\{m_k(s,t),\ k=1,\ldots,K\}$:

$$p(y(s,t)\,|\,m_1(s,t),\ldots,m_k(s,t)) = \sum_{k=1}^{K} w_k N(m_k(s,t),\sigma^2)$$

Observed ozone concentrations are used to estimate σ^2 and the weight parameters for each ensemble member.

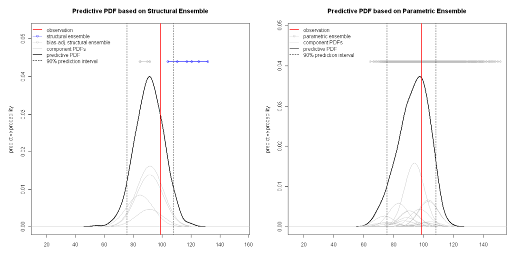


Figure 2. BMA predictive PDF and its components based on the 6 member structural ensemble and 750 member parametric ensemble for the average daily ozone concentrations at a site outside of Atlanta, GA on July 2nd, 2002.

RESULTS

Below is an example of the ensemble predictions at a single site as well as evaluation summary statistics across all of the sites in the study domain. The ensemble generated using CMAQ-DDM-3D reduces the bias in the structural ensemble predictions and has a much higher Brier Skill Score. Post-processing the structural ensemble using BMA based on observed ozone levels produces a similar improvement but has much lower sharpness. Applying BMA to the parametric ensemble produces the best results in terms of lower mean bias and higher BSS.

Case	Structural Ensemble	Structural with BMA	Parametric Ensemble	Parametric with BMA
Mean Correlation	0.74	0.74	0.74	0.76
Mean Error (ppb)	11.9	7.2	7.5	6.8
Spread-skill Correlation	0.39	0.11	0.42	0.35
Brier Skill Score†	-0.06	0.39	0.40	0.46
Reliability*	0.39	0.01	0.06	0.05
Resolution	0.33	0.40	0.46	0.51
Sharpness†	0.46	0.25	0.31	0.28

† Calculated using a threshold concentration of 60ppb.
* A low reliability score implies high reliability.

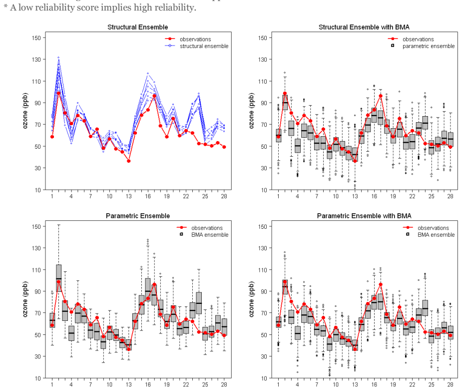


Figure 3. Time series of observed and predicted ozone levels (ppb) at a site outside of Atlanta, GA. Boxplots show the quartiles and the range of the predicted ozone levels for each time period based on structural and parametric ensembles with and without Bayesian Model Averaging.

APPLICATIONS

The ensemble approaches presented here are used to estimate the probability of exceeding an ozone concentration threshold. Below is an illustration for a threshold of 60 ppb daily average ozone. Such information may be used to guide air quality management decisions. Figure 4 shows the reliability of the four different ensembles for predicting this threshold. The parametric and two BMA ensembles show a large improvement in skill over the original structural ensemble. When compared with a single deterministic simulation (Figure 5), these probabilistic estimates provide more detailed information regarding the risk of exceeding the threshold.

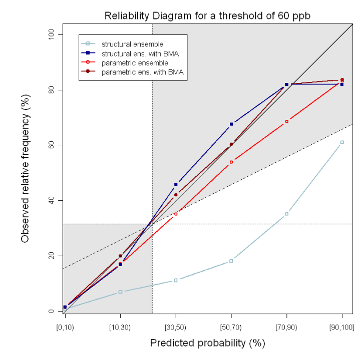


Figure 4. Reliability diagram for a threshold of 60 ppb. The grey shaded area represents ensemble estimates that have overall skill greater than a climatological estimate, denoted by the dotted lines as the observed probability of exceeding the threshold (0.31) .

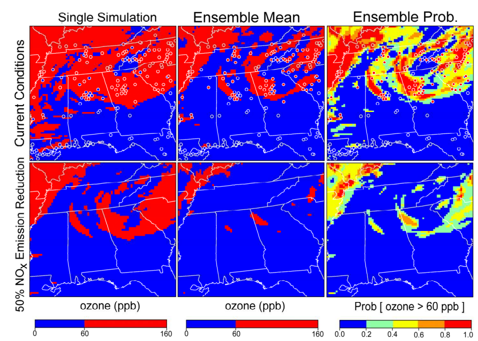


Figure 5. Spatial plots of ozone and probability of exceeding the threshold concentration, for current conditions (top) and with a 50% reduction in NO_x emissions (bottom). These plots are for July 8, 2002 at 5pm EDT. Observations shown in white circles.

DISCUSSION

These methods yield probabilistic estimates with high reliability, resolution, and sharpness. In the absence of quantitative estimates of the uncertainty in the inputs, Bayesian Model Averaging and observed concentrations can be used to significantly improve ensemble skill. Likewise, in the absence of observed values, CMAQ-DDM-3D can be used to efficiently generate ensemble members and improve the ensemble skill. These methods allow air quality managers to quantitatively compare the relative risks and rewards of air quality control options and to select the emissions control strategy that has the largest probability of success.