3.9 Fusing Observations and Model Results for Creation of Enhanced Ozone Spatial Fields: Comparison of Three Techniques

Edith Gégo, P.S. Porter, V. Garcia, C. Hogrefe and S.T. Rao

Abstract This paper presents three simple techniques for fusing observations and numerical model predictions. The techniques rely on model/observation bias being considered either as error free, or containing some uncertainty, the latter mitigated with a Kalman filter approach or a spatial smoothing method. The fusion techniques are applied to the daily maximum 8-hour average ozone concentrations observed in the New York state area during summer 2001. Classical evaluation metrics (mean absolute bias, mean squared error, correlation, etc.) show that fused predictions are not better than a simple interpolation of observations. However, fused maps better reproduce the spatial texture of the model predictions.

Keywords Data fusion, high-resolution maps, ozone

1. Introduction

Because of their adverse effects on human health, a diverse suite of air contaminants is routinely monitored in the United States. Ozone concentrations, for instance, are recorded at more than 1,000 locations. In addition to the rich data base of observations, air contaminant concentrations can be reproduced by photochemical simulation models, numerically transcripting our scientific understanding of atmospheric chemistry and transport processes. The shortcomings of both observational and numerical information are well known. While considered unbiased, ozone measurements are spatially sparse point estimates. Extrapolation of observational information to unmonitored locations leads to smooth spatial images. Maps derived from numerical models, to the contrary, are spatially continuous and detailed but biased. In this context, we compare three simple, flexible and easy to implement techniques for fusing observations and numerical model outputs for the purpose of producing detailed spatial/temporal air contaminant concentration fields that are consistent with both observational and numerical information. Among the potential users of detailed air contaminant information is the public health research community that will be able to refine the exposure fields currently derived from air contaminant observations. The methods are applied to the daily maximum 8-hour average ozone concentrations in a 660 × 828 km rectangular domain centered on

C. Borrego and A.I. Miranda (eds.), *Air Pollution Modeling and Its Application XIX*.

the state of New York, and on the three month period from June 1 to August 31, 2001. Figure 1a shows the domain of interest and the monitoring sites.

2. Ozone Information

2.1. Numerical model estimates

The ozone predictions used in this study were produced by the EPA photochemical simulation system CMAQ (Byun and Schere, 2006). For the application utilized (Appel et al., 2007), CMAQ was set to simulate most of the Eastern United States from January 1–December 31, 2001 with a horizontal grid size of 12 km. Only the predictions for the June 1–August 31 period in the domain of interest, i.e., a block of 55 model rows and 69 columns are utilized here.

2.2. Observations

Measurements collected at 191 sites located within the model domain or in its immediate vicinity (36 km wide strip surrounding the domain) were retrieved from the U.S. EPA Air Data or the NAPS (National Air Pollution Surveillance program of Canada) data bases. The hourly concentrations were used to calculate the daily maximum 8-hour average ozone concentrations for each of the 92 days of interest and each site. Clustered data from sites that fall in the same model cell (15 pairs of sites) were averaged prior to any further operation, leaving a total of 176 'unclustered' locations. Synthetizing the observation and model information, Figure 1 shows the mean of the daily maximum 8-hour average ozone concentration calculated for each site in the domain (panel a) and by CMAQ (panel b) from June 1 to August 31, 2001. Panel c presents the time series of the spatially-averaged averaged 8-hour mean daily maximum concentrations in the domain for the observations and CMAQ estimates. It appears that CMAQ underestimates ozone levels on episodic days, illustrating the need to intregrate model results and observations.

3. Methods

Three simple fusion techniques are considered for this study, all of which aim at determining spatial/temporal bias fields which, when applied to CMAQ predictions, will result in unbiased maps having spatial texture approaching that of CMAQ.

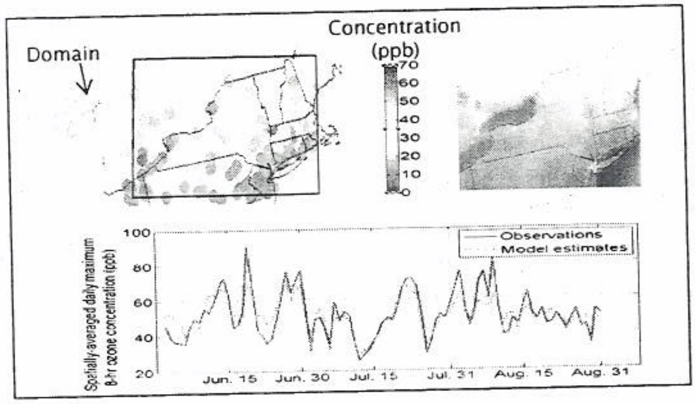

Fig. 1 Site specific (panel a) and CMAQ (panel b) mean daily maximum 8-hour average ozone concentrations during the June 1st to August 31st . 2001 period; Daily mean of daily maximum 8-hour average ozone concentrations (panel c) measured at all 176 locations during the June 1-August 31 . 2001 period (blue line) and CMAQ estimate (red line)

3.1. Method 1: Inverse Distance Weighted (IDW) of bias fields

Method I considers ozone observations error free. Bias is simply defined, therefore, as the difference between model prediction and observation at the 176 monitoring sites. Inverse distance weighting (IDW) method is used to produce spatially continuous 12 × 12 km resolution (CMAQ resolution) bias fields. Fused maps equal CMAQ minus the computed bias field. Preliminary investigation (not included here) showed that the IDW technique led to results as reliable as those obtained by kriging the bias but without the burden of identifying variograms for each simulated day. It also showed that utilizing the ten observations nearest the location being estimated was sufficient to obtain precise estimates.

3.2. Method II: Inverse Distance Weighted (IDW) of Kalman-smoothed bias fields

Method II uses the Kalman filter algorithm (Kalman, 1960) to create an optimal estimate of the true ozone state from observations and model outputs. Primarily designed for time domain applications, the Kalman algorithm recursively estimates a state variable (in this case, model bias) at discrete time increments based on a state equation that describes the temporal evolution of the state variable, and on a series of measurements. Both the state equation and ozone measurements are assumed to be uncertain with respect to true concentrations. The Kalman filter interweaves model and observation uncertainty (var_η and var_ε, respectively) to produce the best linear estimate of the state variable.

The relative strength of the state and observation uncertainties, var_η and var_ε respectively, is a key element of a Kalman filter application. If the measurements are believed more precise than the state estimates, the state estimate will be modified to fit the measurement more closely. Conversely, if the uncertainty of the state equation is insignificant in comparison to that of the measurement, the latter is ignored. In this study, the state variable defines the 'true' correction to be brought to model estimates and its temporal evolution is defined as a random walk. Two scenarios characterize uncertainty. In the first, the ratio of state to measurement variance ($var_\eta var_\varepsilon$ is fixed at 0.06, a value found by Kang et al. (2007) to be optimal for reducing the ozone forecast error of a photochemical model. In the second, $var_\eta var_\varepsilon$ is fixed at 1. The second setting therefore strengthens the correspondence between the estimated state and the measurements while the first setting mostly trusts the state equation. The filter is successively applied to smooth the 92-day time series of observed biases at each measurement location. Following temporal smoothing, fused (spatial) maps are created using the IDW scheme, as in Method 1.

3.3. Method III: spatially-smoothed bias fields

In this scenario, observation/model bias is computed at spatial scales on the order of 200 km. The regional signals are extracted from the original signal using an iterated moving average scheme. More specifically, the calculation window is a 60 × 60 km window (5 × 5 model cells) progressively moved throughout the domain; the averaging process is repeated three times. This method can be seen as the spatial equivalent of the KZ filter originally defined for time series analysis (see Rao et al., 1997 for details). Like the KZ filter, the method can be applied to fields having empty cells, i.e., grid cells that do not contain a monitoring site, an interesting property for treatment of the observations. The correction to be brought to the original model fields are calculated by the difference between the spatially averaged model predictions and the spatially averaged observations.

4. Evaluation of Fused Fields

Comparison of the fused maps generated by the three methods presented above is performed from two perspectives. First, a cross-validation exercise is performed to assess the similarities between the fused data and the original ozone observations. Second, the textures (relief) of the fused ozone fields are compared to those of the initial CMAQ results.

4.1. Calculation of evaluation metrics

The comparability of the fused data with the original ozone observations is assessed using a cross-validation scheme whereby information is omitted one site at time and re-estimated from the remaining data. The procedure is successively repeated for each observation site. The cross validation set up is also utilized to assess the adequacy of ozone concentrations estimated with the IDW method applied to the measurements, hereafter referred to as 'IDW observations'. Strictly speaking, IDW observations are not 'fused'. However, they characterize the quality of maps that are obtained without utilizing model predictions. Mean absolute bias (MAB), root mean squared error (RMSE), and the squared correlation coefficient (R^2) were the metrics of choice in comparing observations and fused data. These statistics were calculated for the ozone predictions generated with the three fusion techniques, as well as for the IDW observations and the original CMAQ estimates, the two latter being good benchmarks.

4.2. Texture comparison of fused maps and CMAQ maps

The evaluation statistics described earlier allow assessment of the quality of ozone predictions at observation sites. However, they do not inform on the texture (relief) of the fields produced, an important feature of spatial information. 'Relief' was defined as the standard deviation of a 60 × 60 km window (5 × 5 grid cells) progressively moved (Increment: 12 km or 1-cell increment) to cover the entire domain. Because of the limited spatial extent utilized for its calculation, the standard deviation computed in this manner is referred to as the local standard deviation.

5. Results

5.1. Evaluation statistics

Table 1 shows the evaluation metrics (MAE, RMSE, R^2) calculated from the 16,192 (92 days x 176 locations) 'estimate-observation' pairs available for each prediction method. The best and poorest values for all three evaluation statistics are found for the IDW observations and CMAQ predictions, respectively. The performances of all fusion methods except Method II utilized with the error ratio $\bar{var}_\eta var_\varepsilon = 0.06$ are quite similar to that of the IDW observations. Table 1 indicates that, although not detrimental, fusion techniques do not lead to better correspondence between predictions and observations than that obtained with IDW of observations only.

Table 1 Evaluation statistics for CMAQ, the interpolated observations (IDW) and the fused predictions.

Statistic	CMAQ	IDW observ.	Fused estimates			
			Method I	Method II $var_\eta/var_\varepsilon=1$	$var_\eta/var_\varepsilon=0.06$	Method III
MAE	9.47	5.81	5.97	7.07	8.67	6.54
RMSE	12.49	8.07	8.49	9.62	11.52	8.35
R^2	0.55	0.81	0.80	0.75	0.62	0.84

A detailed inspection in time and in space of the evaluation statistics indicates that (not shown): (1) spatial-outliers, i.e., locations where measurements stand apart from their neighbours, are least well reproduced, whatever the estimation techniques; and (2) for all techniques, high ozone concentrations days are also high MAE and RMSE days.

5.2. Spatial texture

Figure 2 displays maps of the maximum 8-hour average ozone concentrations predicted by CMAQ and the IDW observations for August 2, 2001 (day chosen at random). Focusing on the texture of each map, one may see that high concentration zones are more sharply delineated by CMAQ map than by the IDW interpolation (Figure 2c and d).

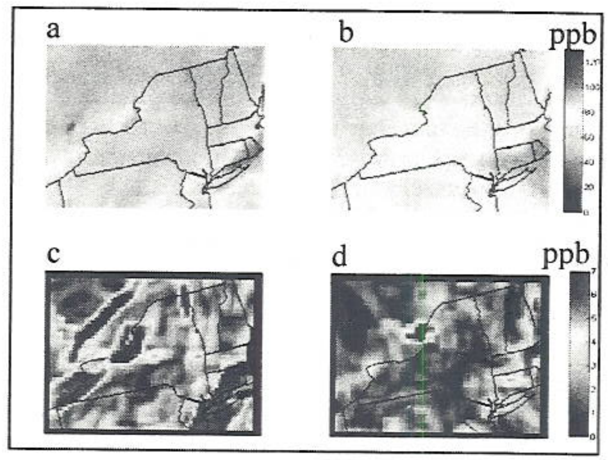

Fig. 2 Map of the predicted maximum 8-hour average ozone concentrations (ppb) for August 2. 2001 by CMAQ (panel a), and by IDW observations (panel b); local standard deviation of CMAQ (panel c) and of the IDW observations (panel d)

Figure 3 shows maps the maximum 8-hour average ozone concentrations predicted by the three fusion techniques for the same day as displayed on Figure 2 (2 August 2001, with method II $var_\eta var_\varepsilon$ = 1) (panels a–c), and the corresponding local standard deviations (panels d–f). All ozone concentration maps (panels a–c) display the relief seen in the original CMAQ estimates combined with the effect of fusing to better fit the observations. High variability zones on panels d and e mostly match those of CMAQ (panel c of Figure 2), meaning that modification of CMAQ values to create fused estimates does not fundamentally alter the basic relief features. It appears that fusing may even have accentuated that relief, probably by establishing ozone levels similar to the observations. Note that the dark spots in panel c correspond to 'empty cells' for which method III did not lead to a numerical value, because these cells are too spatially isolated from any observation site.

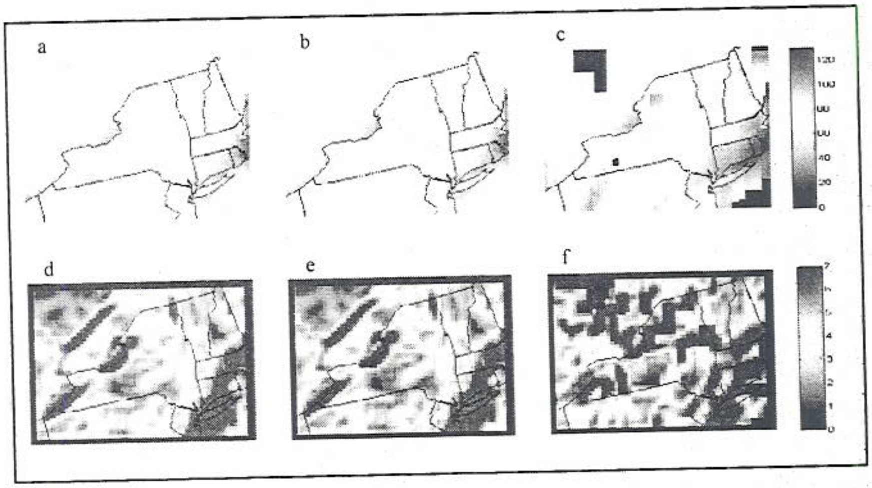

Fig. 3 Map of the predicted maximum 8-hour average ozone concentrations (ppb) for August 2, 2001 obtained by application of fusion method I (panel a), method II (panel b) and method III (panel c) and corresponding local standard deviations (panels d–f)

Generalizing the texture concepts illustrated in Figures 2 and 3 to the entire period, Table 2 presents the overall average (all days and cells included) of the local standard deviations characterizing CMAQ, the interpolated observations and the three fusion techniques, as well as their ratios to the CMAQ mean local standard deviation. The results presented clearly show that spatially interpolating the observations leads to smoother relief than that modeled by CMAQ. To the contrary, the three fusion techniques have a tendency to slightly accentuate CMAQ relief, with Method 2 and CMAQ average relief being remarkably similar.

Table 2 Average local standard deviations of CMAQ, IDW observations and the three fusion techniques and their ratios to the CMAQ mean local standard deviation.

	CMAQ	IDW observ.	Fused results		
			Method 1	Method 2	Method 3
Mean	2.44	1.54	2.76	2.62	3.34
Ratio	1.00	0.63	1.13	1.06	1.36

5. Summary and Conclusion

The objective of this paper is to present three simple techniques for fusing observations and numerical model estimates. Spatial fields were obtained by: (1) spatially interpolating the observed biases with the inverse distance weights method (10 neighbours), (2) spatially interpolating smoothed biases, the Kalman filter being used for the smoothing, and (3) calculating spatially-smoothed bias fields with an iterative moving average technique. The methods were applied to the observed and modeled daily maximum 8-hour average concentrations in a 660 × 828 km domain centered on New York States from June 1 to August 31, 2001. The model estimates were obtained with CMAQ.

The fusion techniques were able to maintain the texture of CMAQ estimates while reducing observation/model bias. In terms of classical comparative metrics (mean absolute bias, the root mean square error and the coefficient of determination between the predicted values and the corresponding observations), fused predictions are not better than simply interpolated observations (IDW method). However, the texture of fused maps is comparable to that of CMAQ in contrast to the smooth nature of interpolated observations.

Disclaimer The research presented here was performed under the Memorandum of Understanding between the U.S. Environmental Protection Agency and the U.S. Department of Commerce's National Oceanic and Atmospheric Administration and under the agreement number DW13921548. This work constitutes a contribution to the NOAA Air Quality Program. Although it has been reviewed by EPA and NOAA and approved for publication, it does not necessarily reflect their policies or views.

References

Appel KW, Gilliland AB, Sarwar G, Gilliam RC (2007) Evaluation of the Community Multiscale Air Quality (CMAQ) model version 4.5: sensitivities impacting model performance: Part I – ozone, accepted for publication in Atmos. Environ.

Byun D, Schere KL (2006) Review of the governing equations, computational algorithms, and other components of the Models-3 Community Multiscale Air Quality (CMAQ) modeling system. Applied Mechanics Reviews, 59, 51–77.

Kalman RE (1960) A new approach to linear filtering and prediction problems, Journal of Basic Engineering, 82, 35–45.

Kang D, Mathur R, Rao ST, Yu S (2007). Bias-adjustment techniques for improving ozone air quality forecasts, Journal of Geophysical Research, in review.

Rao ST, Zurbenko IG, Neagu R, Porter PS, Ku JY, Henry RF (1997) Space and time scales in ambient ozone data, Bulletin of the American Meteorological Society, 78, 2153–2166.