A MODEL PERFORMANCE EVALUATION SOFTWARE: DESCRIPTION AND APPLICATION TO REGIONAL HAZE MODELING

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1. INTRODUCTION

Particulate matter (PM) models are used for demonstration of progress in visibility under the Regional Haze Rule and the formulation of State Implementation Plans (SIPs) for the $PM_{2.5}$ National Ambient Air Quality Standards (NAAQS). For models to be used convincingly in the regulatory arena, they must first be shown to produce satisfactory performance[1, 2]. The evaluation of models is a data-intensive activity, requiring PM and precursor data from many networks. To facilitate data retrieval and formatting for model evaluation activities, a Model Performance Evaluation (MPE) software has been developed that includes a database of relevant air quality data as well as software for the calculation of a large array of model performance statistics. The MPE software retrieves the relevant air quality data and model simulation outputs and calculates performance metrics selected by the user. We first describe the MPE software package. Next, we present an application for regional haze modeling.

2. DESCRIPTION OF THE MODEL PERFORMANCE EVALUATION SOFTWARE

2.1 Design Principles

Model evaluation is a complex activity, because models can be evaluated in many ways, including the use of a variety of statistics and displays. Another dimension of complexity is added to PM model evaluation because, in most instances, the evaluation also involves PM composition, precursor gases, and deposition fluxes. Therefore, the MPE software needs to be flexible but not cumbersome. To keep the design simple, the software package evaluates one species at a time. (A shell script can be used to repeat model evaluation for multiple species using different input files.) Thus, specific procedures and options can be applied to specific species. For example, a different threshold can be used for gases vs. particulate species. As described below, options are provided in the software, and the selection of these options is made in a user control file.

1.1 Software Engineering Standards

Under the ISO 9001 quality system, AER incorporates specific procedures for configuration management and software standardization that are consistent with the Carnegie Mellon Software Engineering Institute standards. The model evaluation software is written in Fortran 90 (ANSI standard) with Models-3 I/O-API directives. The MPE software is well documented using comments within the code. A user's guide is available that describes the inputs, functionalitites, architecture, and outputs of the software[3].

2.3 Model Output Data

The MPE software requires input of model results in NetCDF format. Time-varying two-dimensional (surface layer) or three-dimensional (x, y, z) NetCDF files are used as input to the MPE software for chemical species deposition and concentration. For PM fractions, the NetCDF file needs to contain both the PM component and total $PM_{2.5}$ mass. CMAQ and CMAQ-MADRID three-dimensional output files can be used directly for model performance evaluation. The surface layer can also be extracted (using the NetCDF function m3xtract) to reduce the input/output burden.

A Fortran preprocessor is also provided with the MPE package. The main function of the preprocessors is to convert binary output from CAMx to NetCDF format. The model output files that are converted are the two-dimensional hourly average file and the deposition file. A secondary function is to aggregate PM and wet deposition species to facilitate analysis and model evaluation.

The MPE software performs all the necessary steps needed to match model outputs to monitoring data. Such steps include identifying the grid cell corresponding to the latitude and longitude of a given monitoring site, extracting the model output for that grid cell, summing model components to match a measurement variable and performing unit conversions.

2.4 Meteorological Data

Meteorological data, namely temperature and pressure, are needed in the event that a unit conversion is needed between mixing ratio and concentration units. If wet deposition is to be evaluated in terms of liquid concentration, the model output of deposition flux needs to be divided by the amount of precipitation to calculate concentrations. In these cases, the meteorological data used in the execution of the model should be supplied to the MPE software.

For CMAQ and CMAQ-MADRID model data, MCIP output is already in NetCDF format. Meteorological data are converted from binary format to NetCDF format where necessary, e.g., for CAMx. A preprocessor is provided to accomplish the conversion from binary data to NetCDF for those meteorological variables needed in the model evaluation software.

2.4 Air Quality Data

The air quality data are available in a database written in MySQL. This database includes data from the IMPROVE, CASTNet, AQS and SEARCH ambient networks and NADP and MDN deposition networks. Those data are available in their original databases in different formats. The MySQL database provides all these data under a common format. In addition, supporting information such as site location, sampling start time (including time zone), sampling duration and units are available within the database. The MPE software retrieves the needed air quality data from the database and performs the required processing steps including time averaging, time zone adjustments and unit conversions.

The options available to the user in terms of species treated in the model performance evaluation include $PM_{2.5}$ and PM_{10}, $PM_{2.5}$ components (sulfate, nitrate, ammonium, organic carbon and elemental/black carbon), $PM_{2.5}$ fraction (this requires collocated measurements of $PM_{2.5}$ and $PM_{2.5}$ components), gases (O_3, NO_x, NO_y, VOC and SO_2) and wet deposition (both concentrations in precipitation and deposition fluxes).

2.5 Processing Options

The user can select from several options when conducting the model performance evaluation.

Subdomain options: The user can conduct the evaluation for the entire modeling domain or by subdomains. Those subdomains can be defined in many different ways (lists of sites (e.g., for certain metropolitan statistical areas), longitude/latitude, groups of grid cells).

Temporal options: The user can select a subperiod within the modeling period. Temporal averaging can be performed (it must be equal to or greater than the measurement sampling period).

Spatial processing options: Several options are available to the user when comparing grid cell results to measurement point values. Such options include using a single grid cell value, linear interpolation using the four closest grid cells, averaging neighboring grid cells, best estimate from neighboring grid cells and distance-weighting among neighboring grid cells.

Statistical options: The threshold for selecting measured values used in the evaluation is specified by the user for each chemical species. Statistical metrics that can be used include accuracy of peak (unpaired in time; paired and unpaired in space), mean observed and modeled values, gross and normalized bias and error, coefficient of correlation (r), normalized root mean square error, ratio of means, fractional bias and error, coefficient of determination (r^2), index of agreement, site specific root mean square error, and normalized mean bias and error.

3. EXAMPLE OF AN APPLICATION OF THE MPE SOFTWARE

The MPE software has already been applied in many air quality studies. We present here an example of its application for the modeling of regional haze in Big Bend National Park, Texas, that was conducted with CMAQ-MADRID as part of the BRAVO study[4]. This example evaluation uses data from the IMPROVE, CASTNet and AQS monitoring networks.

CMAQ-MADRID was applied to a domain that covered Texas, surrounding states and part of northern Mexico with a spatial resolution of 36 km. A four-month period (July-October 1999) was simulated. Figure 2 presents some model performance evaluation results.

4. CONCLUSION

We have presented the development and application of a new Model Performance Evaluation (MPE) software that allows air quality modelers to evaluate the performance of air quality models with a large array of air quality data in an effective manner. The MPE software is currently compatible with CMAQ, CMAQ-MADRID and CAMx, and it can easily be adapted for other models. It is publicly available and is distributed by CMAS (http://www.cmascenter.org).

ACKNOWLEDGEMENTS

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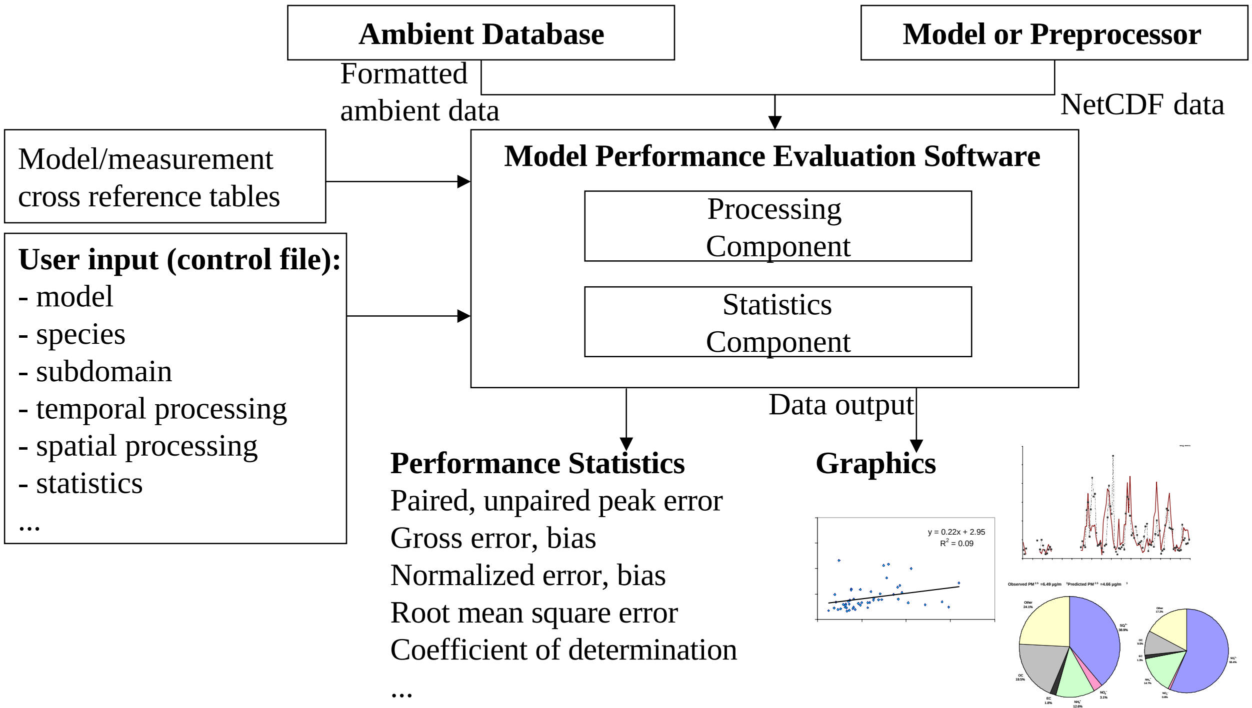

Figure 1. Schematic description of the MPE software and associated air quality database.

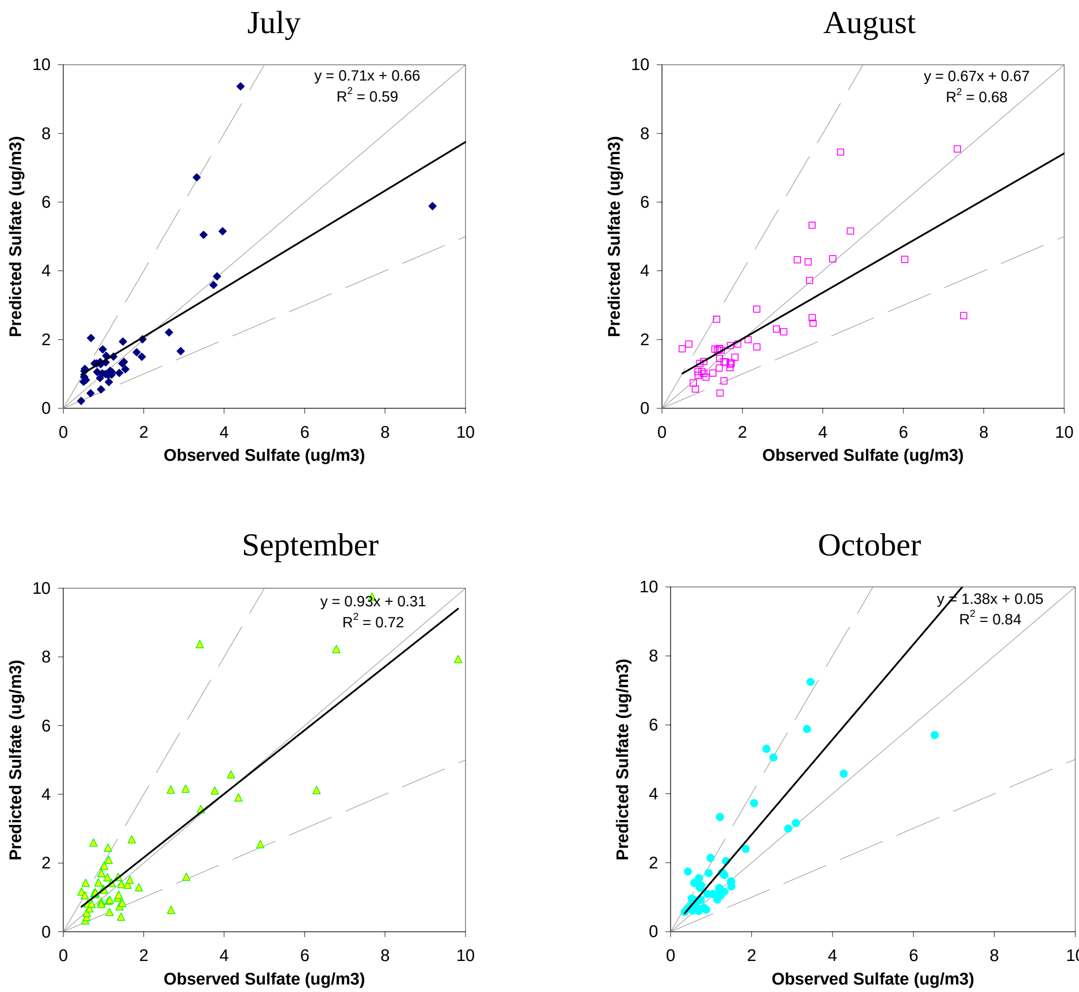

Figure 2. Examples of model performance evaluation for the CMAQ-MADRID simulation of regional haze in the BRAVO study[4]