Emission Processing for an Air Quality Forecasting Model

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ABSTRACT

The creation of emission data for a photochemical quality-forecasting model requires the efficient and accurate estimation of temporal and spatial variations of emission sources of ozone precursors. To achieve this goal, the existing emission inventory preparation and processing systems need to be streamlined and modified. The critical emission precursor pollutants for ozone are volatile organic compounds (VOCs), nitric oxides (NOx), and carbon monoxide (CO). The spatial variability and temporal behavior of these compounds are influenced both by meteorological conditions and by anthropogenic activities. The key complexities in the simulation of the temporal and spatial variations of these compounds are the biogenic sources, the on-road mobile sources, and major fossil-fuel point sources. The processing of the emission for biogenic sources can be streamlined by linking the preparation of meteorological output fields for the air quality chemistry model with the calculation of biogenic emission. The processing of temperature-dependent emission for mobile sources can be streamlined by using the MOBILE5B (or MOBILE6) model to create simple temperature regressions to apply to normalized emission data prior to the actual forecast. The temperature/emission relationship can then be used in a very efficient calculation for the actual emission calculation. Finally, the processing of point source emission from major power plants can be streamlined by using historical CEM (Continuous Emission Monitoring) data to create temperature/emission relationships that can be used to estimate current power plant emission in an air quality forecast model. This streamlined approach will be compared to the typical emission processing method used in a non-operational environment.

INTRODUCTION

The U. S. Environmental Protection Agency in cooperation with the National Weather Service is developing a National Air Quality Forecasting System to provide timely forecasts of ozone, particulate matter, and other pollutants to prevent or reduce adverse effects of these hazards. The planned capabilities of the modeling system can be divided into the initial phase, the medium-term plan, and the long-term plan. The initial capability of the system is to develop and validate 1-day forecasts of ozone (O_3) for the Northeastern US and expand nationwide within 5 years. The medium-term (5-7 years) goal is the development and deployment of a nationwide capability to forecast particulate matter concentration for particulate size less than or equal 2.5 microns (PM 2.5). In the long-term plans (within 10 years), the forecast range of the air quality system will be extended to 48-72 hours and include a broader range of significant pollutants.

For the Initial Operating Capability (IOC), the target deployment is September 14, 2004 for the Northeast US with one-day ozone forecasts. Hourly ozone concentrations and an eight-hour average of ozone in parts per billion (ppb) will be forecast for the surface layer. Forecasts at additional vertical levels of 50 meters and 500 meters above the surface will be added. The forecast will be delivered twice

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daily. The primary forecast for the following day will be delivered by 1730 Coordinated Universal Time (UTC) and will be valid for 24 hours through 4 UTC day 3. The updated forecast will be for the current day and will be delivered by 1300 UTC and will be valid for 15 hours through 4 UTC, day 2. The National Weather Service will be responsible for the operational forecasts while the EPA will be developing the modeling system. These operational requirements specify that the post-processing of the meteorological data, the emission processing and air quality chemistry model simulation be completed in less than five and a half hours. Since the post-processing of the meteorological data and the air quality chemistry model are typically very time consuming, the emission processing time needs to be minimized to less than 15 minutes per run. A typical emission-processing scenario in a research environment on a national domain for one day takes up to 3 hours of time on a single CPU. Therefore, in an operational environment, the emission processing needs to be streamlined with all non-meteorological dependent operations completed well in advance of the forecast. Only the meteorology dependent component of the emission processing needs to be done operationally. The accuracy of the emission processing can be maintained and the forecast can be completed within the required time constraints.

EMISSION PROCESSING SYSTEM

An emission processing system requires meteorological inputs, an emission inventory, and other ancillary input files. This information is used to do temporal allocation, spatial allocation, and chemical speciation of the emission inventory to create time-dependent gridded input for an air quality model. An emission processing system requires both meteorologically dependent inputs (such as wind and temperature) as well as static non-meteorological inputs (spatial surrogates, land use data, emission inventories). These inputs are used independently by different components of the emission processing resulting in many opportunities for parallelism. In an operational environment, the non-meteorological component of the emission processing can be separated from the meteorological component thereby reducing the amount of processing that has to be done on an operational basis.

Our approach to emission processing for an air quality forecasting system is to split the emission processing into two parts: the meteorologically dependent component and the non-meteorologically dependent component. The meteorologically independent part includes stationary area source processing, non-road mobile source processing, the calculation of normalized biogenic calculations, the calculation of temporal factors, speciation factors, and grid factors for point sources, and the temperature-independent component of mobile source processing. The emission processing system to be used for air quality forecasting is SMOKE[1] (Sparse Matrix Operator Kernel Emission). SMOKE uses high performance computing sparse matrix algorithms. The sparse matrix approach permits rapid and flexible processing of emission data[2]. Processing steps are separated into independent operations wherever possible. The meteorologically independent calculations can be done with the existing programs within SMOKE except that the temperature dependent component of the mobile source processing cannot directly be separated from the rest of the mobile source processing. SMOKE creates mobile source emission factors with MOBILE5b for a wide variety of exhaust and evaporative processes and pollutants. MOBILE5b is a vehicle emission factor model, which is a software tool for predicting gram per mile emission of hydrocarbons (HC), carbon monoxide (CO), oxides of nitrogen (NOx), carbon dioxide (CO_2), particulate matter (PM) and air toxics from cars, trucks, and motorcycles under various conditions.[3] The MOBILE5b model has been integrated into SMOKE. All future releases of SMOKE will include integration with the latest mobile source emission model (Mobile6). The discussions here with respect to MOBILE5b are also applicable for Mobile 6. MOBILE5b inputs include an ongoing inspection/maintenance programs, reformulated gasoline, vehicle registrations, fuel volatility parameters, vehicle speeds, and temperature. Therefore, mobile source emission processing becomes more complex than any of the other source processing.

We will focus our attention first on the mobile source processing, since the meteorological component (i.e. the temperature dependence) is an intrinsic part of the MOBILE5b model and we wish to separate this dependence from all the other parameters in the SMOKE/MOBILE5b system. Our emission processing system (SMOKE) uses the MOBILE5b model to estimate mobile source emission from vehicle activity data.

For mobile source emission, we propose to separate the temperature dependence of the mobile source emission processing from all other non-meteorological dependencies in the SMOKE/MOBILE5b by running the SMOKE/MOBILE5b model in two different modes. First, using a reference temperature of 75 F, (the temperature at which mobile source emission are minimum in the MOBILE5b model[4]), the SMOKE/MOBILE5b model is used to create emission estimates for the modeling period assuming a constant temperature. The emission factors generated under this assumption capture the speciation, the temporal factors due to anthropogenic activity, and the vehicle fleet information for each grid cell in the domain. These normalized emission factors are then saved for future use. Second, a flag in the SMOKE/MOBILE5b model allows the temporal factors to remain constant for all hours. Using this flag, the temperature only dependence can be estimated for each grid cell if ambient temperature data are available for some past time period. Using historical temperature data, emission factors that are only dependent on temperature are calculated. Next, we use a nonlinear least squares approach to create a relationship between temperature and emission rates for each grid cell and for each time step:

$$E_s(x,y,t) = f_s(x,y,T(t),T_0)\,. \tag{1}$$

In Equation (1), T is the temperature at the grid cell, T_0 is a reference temperature and s is a chemical species (e.g. NO) from the chemical mechanism of the air quality model. We approximate the relationship between an emission rate and temperature by doing a nonlinear least squares fit to the temperature and emission rates. We only need to determine the function $f_s(x,y,t,T,T_0)$ for each model species at each grid cell. For carbon monoxide (CO), we use a sixth order polynomial:

$$\begin{aligned} f_{CO}(x,y,T(t),T_0) &= a_6(x,y)(T(t)-T_0)^6 + a_5(x,y)(T(t)-T_0)^5 \\ &+ a_4(x,y)(T(t)-T_0)^4 + a_3(x,y)(T(t)-T_0)^3 \\ &+ a_2(x,y)(T(t)-T_0)^2 + a_1(x,y)(T(t)-T_0) \\ &+ a_0(x,y) \end{aligned} \tag{2}$$

For NO, and NO_2, we use a piecewise linear function that is continuous at the reference temperature:

$$f_{NOX}(x,y,T(t),T_0) = \begin{matrix} a_1(x,y)(T(t)-T_0) + a_0(x,y), T(t) \geq T_0 \\ a_2(x,y)(T(t)-T_0) + a_0(x,y), T \leq T_0 \end{matrix} \tag{3}$$

For Volatile Organic Compounds (VOCs), we use a quadratic function given by

$$f_{VOC}(x,y,T(t),T_0) = a_2(x,y)(T(t)-T_0)^2 + a_1(x,y)(T(t)-T_0) + a_0(x,y) \tag{4}$$

VOC emission are calculated by MOBILE5b for several emission forming processes: exhaust VOC emission, evaporative VOC emission which is the sum of "hot soak", "crankcase", and "weighted diurnal emission", "resting loss" VOC emission, "running loss" VOC emission, and "diurnal" VOC emission. "Exhaust" emission are from the tailpipe of the vehicle. "Running loss" emissions are evaporative emission not accounted for by other processes. "Resting Loss" evaporative emission are from resting vehicles, representing the time period after the hot-soak is complete, but not associated with

diurnal temperature variation. "Weighted diurnal" emissions represent evaporative emission from carbon canisters that have been sitting for a partial day, full day, or multiple days. "Diurnal" emissions are evaporative emission due entirely to diurnal variations in temperature. MOBILE5b uses only the minimum and maximum temperature during the day to estimate this component. "Crankcase" emissions are evaporative emission emanating from the crankcase of a vehicle.

The nonlinear least squares calculation is performed using the temperature only dependent emission factors and the temperature field for each species and for each grid cell in the domain for a sufficient time period of available meteorological information. The coefficients $a_0, a_1, a_2, a_3, a_4, a_5, a_6$ for each grid cell are stored. These coefficients together with the prescribed functions for each species and normalized emission factors calculated previously are then combined to generate the operational estimate of the mobile source emission according to:

$$E_s(x, y, t, T, T_0) = \frac{f_s(x, y, T(t), T_0) \cdot g_s(x, y, t)}{f_s(x, y, T_0)} \tag{5}$$

This final emission calculation is extremely fast and is the only part of the mobile source emission processing that has to be performed operationally.

The nonlinear least squares calculation is undertaken with MINPACK[5]. MINPACK is a free, portable library for solving nonlinear systems of equations and nonlinear least squares problems. The specific algorithm from MINPACK uses an analytic specification of the Jacobian matrix and minimizes the sum of the squares of the nonlinear functions by a modification of the Levenberg-Marquardt algorithm[6]. This algorithm is well suited to this problem since it allows the user to provide the subroutine, which calculates the analytic functions and the Jacobian of the analytic function.

For biogenic emission calculations, the Biogenic Emission Inventory System[7] (BEIS) is already computationally very fast. Therefore, only minor adjustments to streamline this component of the emission processing are required for air quality forecasting.

For point source emission calculations, the plume rise method is meteorologically dependent. In addition, CEM (Continuous Emission Monitoring) information from power plants is not available in real time. Therefore, the temporal factors for SO_2 and NO_x from power plants will be estimated in the same way the other pollutants and other sources without CEM data are estimated. Temporal factors dependent on the Source Classification Code (SCC) of the point source will be used in the air quality forecast system. Since the plume rise calculation is meteorological dependent, this calculation will be performed operationally for each point source. Should this calculation require too much time for all point sources, this calculation could be simplified and only applied to the larger sources. We propose to use the plume rise calculation in SMOKE in the meteorological component of the emission processing. However, the mapping of the point sources to grid cells, the temporal factor calculations, and speciation can be done and stored in matrices in advance of the operational component of the emission processing.

PRELIMINARY RESULTS

We will focus on the nonlinear least squares approximation applied to mobile source emission for a 32km continental domain for a June 12-30, 1999 time period. Using the methodology described above, we will first examine a single 32km grid cell of Atlanta, GA for this time period and compare the MOBILE 5B emission rates calculated with SMOKE with the emission rates computed using the nonlinear least squares approximation.

Figure 1 shows the relationship between the CO emission rate and temperature for both SMOKE/MOBILE 5B and a sixth order polynomial least squares approximation for every hour for the period of June 12-30, 1999. We note the minimum in the emission rate at approximately 297°K (75°F). A minimum emission rate at 75 degrees is built into the MOBILE5b model. After application of the nonlinear least squares method to all grid cells for the entire time period and summing up the emission for each 24 period, we are able to see the accuracy of the nonlinear least squares method. Figure 2 shows the domain totals for the continental US for each day from June 12 to June 30, 1999 for CO. We see that the nonlinear least squares approximation for the emission is consistently lower by 1- 2% each day compared to the emission from SMOKE/MOBILE5b.

For NO and NO2 emission, a piecewise linear function was used to approximate the temperature dependence of the mobile source emission. Figure 3 shows the emission rate as a function of temperature for a single 32km grid cell of Atlanta, GA for NO. Figure 4 shows the domain totals for NO for the continental US for each day from June 12 to June 30, 1999. We see that the least squares approximation for the emission is in very good agreement, less than 0.2% difference between the Mobile 5B emission and the least squares approximation.

For VOC emission, a quadratic function was used to approximate the temperature dependence of the mobile source emission. We use a quadratic function for all VOC species since MOBILE5b calculates VOC emission directly. MOBILE5b calculates VOC emission for several emission forming processes as indicated previously. We created separate functions for each VOC species related to the chemical mechanism to be used in the air quality model. This simplifies the mobile source calculation that is done operationally since chemical speciation, spatial allocation, and temporal allocation can all be included in the mobile source emission factors. We look at the temperature dependence of the emission rate from one VOC species, paraffin (PAR), from the carbon-bond-four (CB4) chemical mechanism. Figure 5 shows the emission rate of paraffin as a function of temperature for a single 32km grid cell of Atlanta GA. We note that there is more variation in the emission rate for a single temperature. This is likely due to fact that all the VOC emission-forming processes are considered as a group. Figure 6 shows the domain totals for PAR for the continental US for each day from June 12 to June 30, 1999. The difference between MOBILE5b and the nonlinear least squares approximation is on the order of 3 – 4 %.

CONCLUSIONS

The separation of the meteorologically dependent component from the non-meteorologically dependent component of emission processing is crucial to the development of a rapid, operational emission processing system for an operational air quality forecast system. The meteorological dependence of mobile source emission in the MOBILE5b model and the complex nature of the MOBILE5b model requires the development of an approximation to the MOBILE5b model that is very fast computationally, although not as accurate as the MOBILE5b model itself. We have demonstrated that the use of a nonlinear least squares approximation of the dependence of emission rates to temperature can allow for a very fast, yet approximate method for calculating mobile source emission in an air quality forecasting model. The nonlinear least squares method produces emission totals that are within 5% of the emission totals generated with the MOBILE5b model at a fraction of the computational time. The emission processing in an air quality forecast system could be computationally fast and efficient by separating the meteorological dependent component of the emission processing from the non-meteorological dependent component. A nonlinear least squares method can be used to approximate the temperature dependence of mobile source emission. Biogenic emission calculations can be incorporated directly into the operational component of the emission processing. Only the plume rise component of the point source emission processing is done operationally in the emission processing.

Figure 1 CO Mobile source emission for one 32km grid cell as a function of temperature

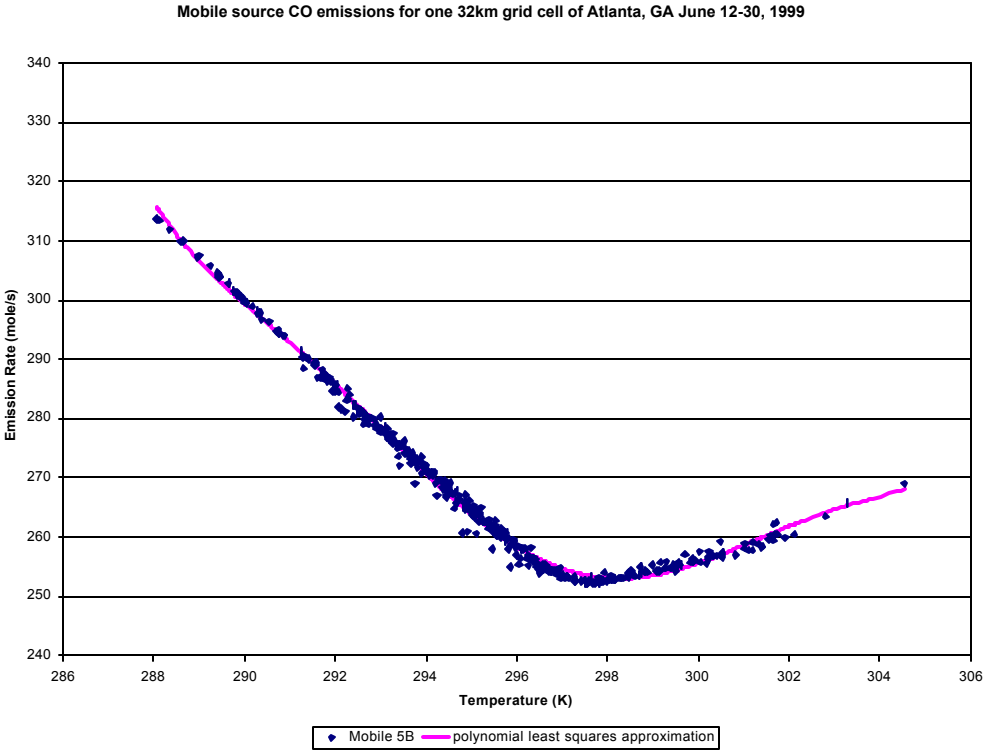


Figure 2 CO domain totals for June 12-30, 1999

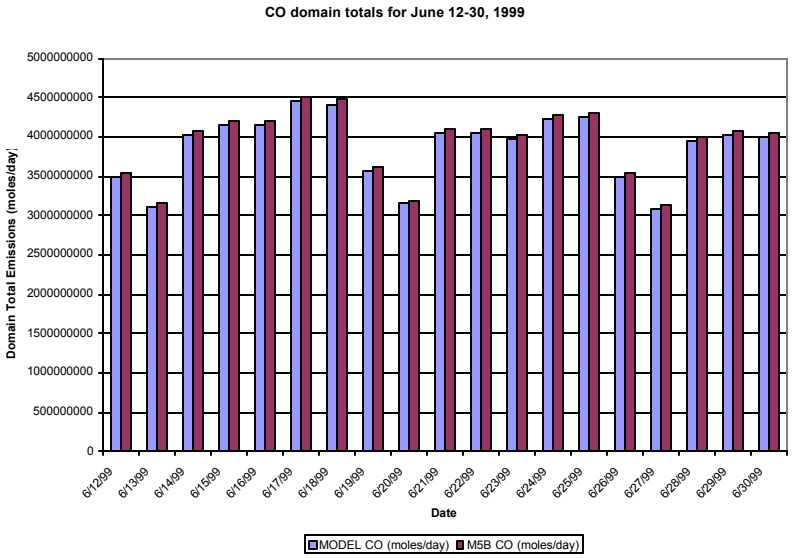


Figure 3 NO Mobile source emission for one 32km grid cell as a function of temperature

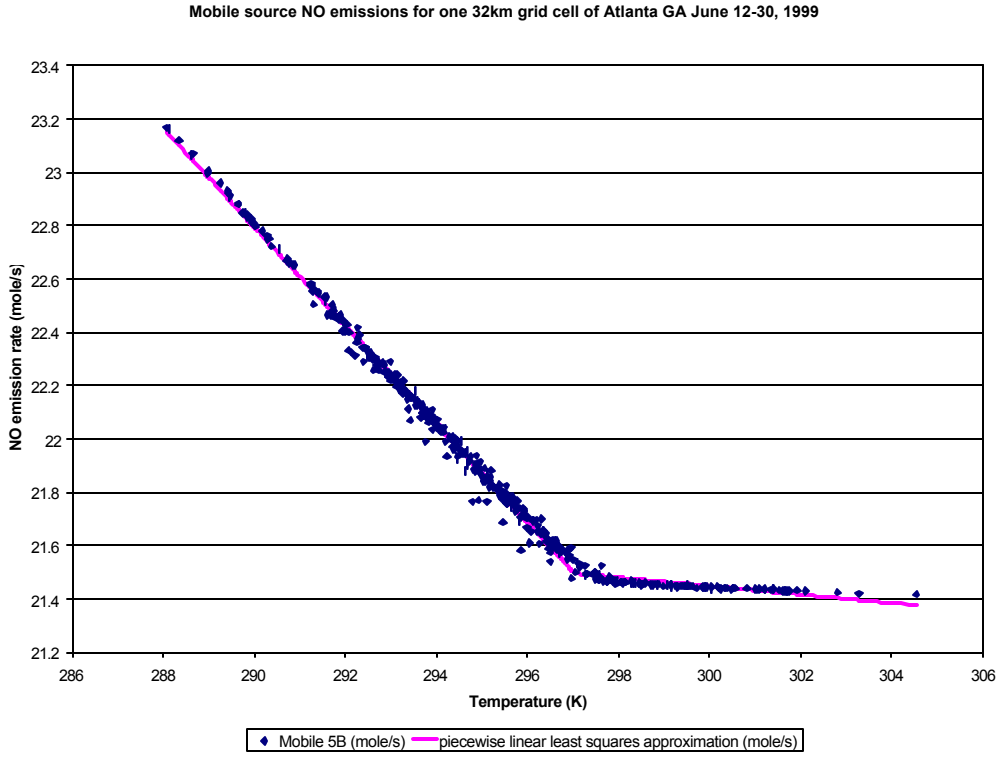


Figure 4 NO domain totals for June 12-30, 1999

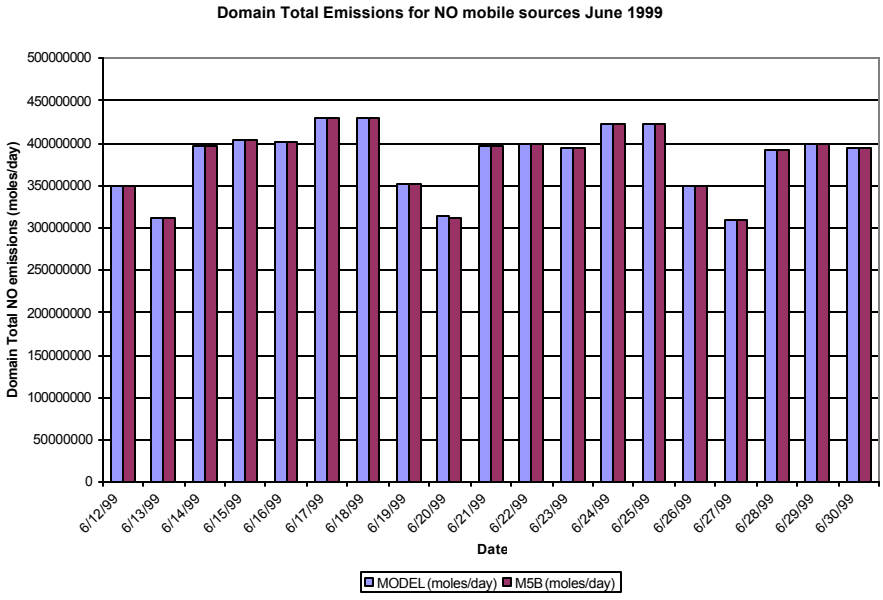


Figure 5 PAR Mobile source emission for one 32km grid cell as a function of temperature

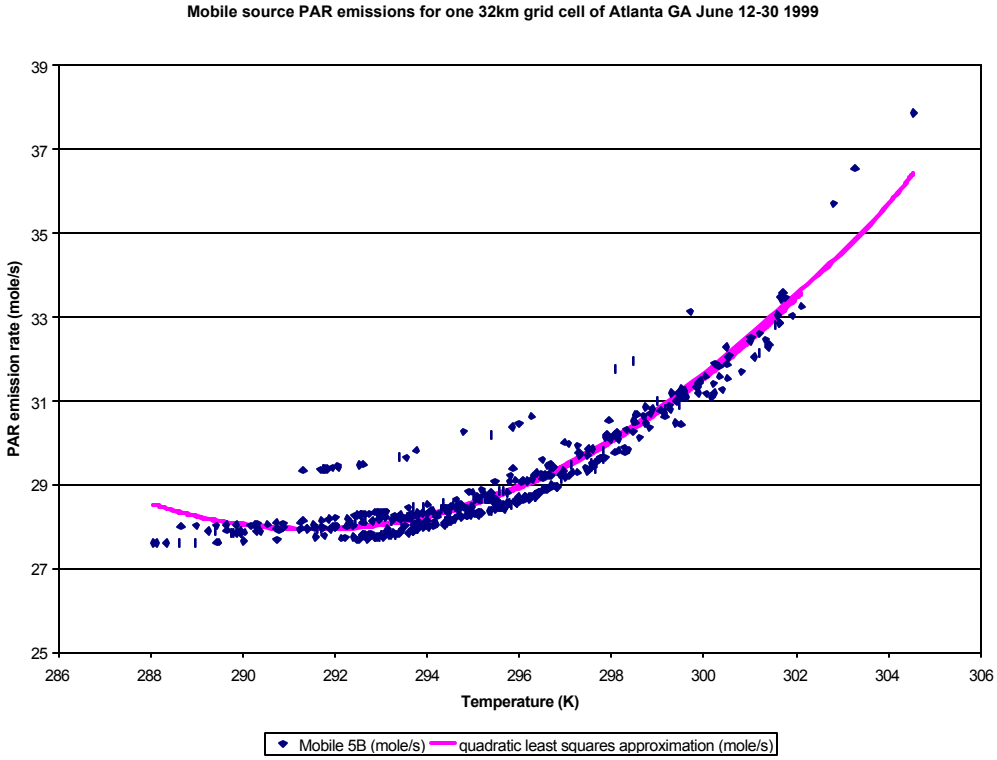
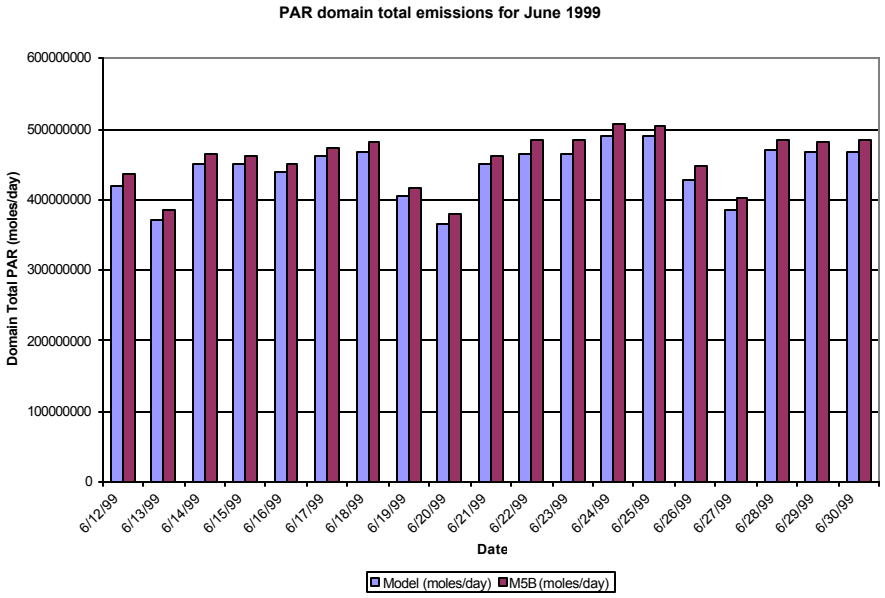


Figure 6 PAR domain totals for June 12-30, 1999



DISCLAIMER

This paper has been reviewed in accordance with the U.S. EPA peer and administrative review policies and approved for presentation and publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for their use.

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KEYWORDS

Emission Modeling
Air Quality Forecasting