

IMPLEMENTATION OF THE PARTICLE AND PRECURSOR TAGGING METHODOLOGY (PPTM) FOR CMAQ

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1. INTRODUCTION

To improve the utility of the CMAQ modeling system (EPA, 1999; CMAS, 2006) for the study of fine particulate matter (PM_{2.5}) and the identification of effective PM_{2.5} control strategies, we have enhanced the model to include the Particle and Precursor Tagging Methodology (PPTM). This methodology is designed to provide detailed, quantitative information about the contribution of selected sources, source categories, and/or source regions to simulated PM_{2.5} concentrations. Emissions from selected sources, source categories, or source regions are (numerically) tagged and then tracked throughout a simulation. The contribution from each tag to the resulting simulated concentration of PM_{2.5} or its component species for any given location can be quantified. By tracking the emissions from selected sources or source locations, the methodology also provides information on the fate of the emissions from these sources.

The tagging methodology differs from the use of sensitivity simulations in which the emissions are modified or eliminated (zeroed-out). Sensitivity simulations typically provide information about the effects of changes in the emissions on the simulation results. In contrast, tagging provides information about the contribution (or fate) of the emissions from the tagged sources, relative to the unmodified simulated conditions. Identifying and quantifying source contributions and tracking the fate of emissions from certain sources or source sectors is important in air quality planning.

The CMAQ Particle and Precursor Tagging Methodology (PPTM) currently includes sulfur, nitrogen and mercury tagging. Tagging for organic and elemental carbon species and other inorganic particulates is currently under development. PPTM

has been incorporated into version 4.5 of CMAQ. PPTM was first developed by ICF in 1999 and was incorporated into the Regional Modeling System for Aerosols and Deposition (REMSAD), for the EPA Office of Water (OW). A detailed technical description is included in the REMSAD user's guide (SAI, 2005). Thus, prior to incorporating the methodology into the CMAQ model, PPTM has been extensively tested and applied within the context of the REMSAD model. A similar methodology (Ozone and Precursor Tagging Methodology (OPTM)) has also been used for oxidant tagging in the UAM-V modeling system. This paper describes the implementation and testing of PPTM for sulfur (SO₂ and emitted particle sulfate) and nitrogen. A discussion of mercury tagging capabilities for CMAQ is offered in a separate paper and is described in some detail by Douglas et al. (2006).

2. OVERVIEW OF THE METHODOLOGY

The CMAQ Particle and Precursor Tagging Methodology (PPTM) is designed to tag and track the release, transport, chemical transformation, and deposition of precursor species from emission sources, source categories, or source regions within the modeling domain, and to determine the contributions of these emissions to simulated particulate concentrations and deposition at any given location and time. Multiple sources, source categories, or source regions can be tagged in a single CMAQ simulation.

The advantage of the PPTM is that it can readily answer questions regarding source contributions to identified receptors or receptor regions. The PPTM can provide daily, seasonal, and annual average contributions and can be used to determine whether annual contributions from a particular source or source category are dominant in one season or another. In addition to providing information regarding the magnitude of contribution, it can also answer questions regarding the range of influence, including interstate transport, of emissions from a

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source/source region on simulated downwind $PM_{2.5}$.

Within the model, tagging (PPTM) is accomplished by the addition of duplicate model variables for each species and tag (e.g., SO_2_{t1} , SO_2_{t2} , etc. or NO_{t1} , NO_{t2} , etc.). The tagged species have the same properties and are subjected to the same processes (e.g., advection, chemical transformation, deposition) as the actual (or base) species. Because the tagged species are separate from the base species, PPTM does not alter or affect the base simulation results.

At each time step in the simulation, the effects of linear processes, such as advection and dry deposition, are calculated directly for all tagged species. Potentially non-linear processes, such as gas-phase chemistry, aqueous chemistry, and particle dynamics are calculated for the overall (or base) species and apportioned to the tagged species. The results for the tagged species are not normalized to ensure that the sum of the tagged species equals the total. Thus, the difference between the sum of all tags and the overall concentration gives an estimate of the numerical uncertainty in the contribution estimates. Due to the number and type of chemical reactions PPTM sulfur is more complex than that for mercury, and PPTM for nitrogen is more complex than that for sulfur.

Some example uses of the PPTM methodology for sulfur and nitrogen include:

- quantifying the contribution of emissions from various source sectors (e.g., power plants, pulp and paper mills, chemical manufacturing facilities, and motor vehicles) to $PM_{2.5}$ concentrations at selected locations throughout the modeling domain,
- quantifying the contribution from boundary conditions to $PM_{2.5}$ concentrations throughout the modeling domain,
- examining the range of influence of emissions from selected facilities or geographic regions, and
- tracking the fate of emissions from specific facilities or geographic regions to estimate their contribution to $PM_{2.5}$ concentrations in nonattainment areas throughout the modeling domain.

3. SUMMARY OF APPLICATION PROCEDURES

The first step in the application of PPTM is to identify the sources that are to be tagged, both in concept as well as within the emission inventory (e.g., by Source Identification Code (SIC), location, etc.). For each simulation, it is necessary for all contributing elements (emissions, initial conditions, boundary conditions) to be tagged. This is usually accomplished by tagging selected elements and then including all other elements in a final ("all other") tag. This allows the user to estimate the numerical uncertainties associated with the contributions.

The next step is to prepare the tagged emissions and/or initial/boundary condition files. These are prepared in the same manner as the ordinary input files, but the tagged species are given different names (e.g., SO_2_{t1} , SO_2_{t2} , etc.) than the original species. A utility program is available to support the preparation of these files. The tagged emissions are then merged with the remaining emissions and the CMAQ model is run as usual.

The tagged species are included as additional species in the model output files and the results can be postprocessed and displayed using any standard CMAQ postprocessing software. Spatial plots of the tagged species can be used to show the extent and magnitude of the contributions from the tagged sources within the modeling domain. The contribution from each tag at individual locations throughout the domain can also be extracted from the gridded model output. Finally, the tags can be summed and compared with the base simulation results to quantify the numerical accuracy of the results.

4. EXAMPLE FOR SULFUR TAGGING

PPTM for sulfur has been incorporated into version 4.5 of CMAQ. Modifications to CMAQ involve several existing subroutines and INCLUDE files, as well as the addition of new subroutines and INCLUDE files. The tagged elements for sulfur tagging include sulfur dioxide (SO_2) and particulate sulfate.

To illustrate the sulfur tagging methodology, we tagged the emissions from three individual facilities in the Southeast (specifically in Tennessee and South Carolina) and applied CMAQ for a one month period in July 2002. An

early version of the VISTAS regional planning organization CMAQ modeling database was used for this example analysis.

Spatial plots (Figure 1) show the contribution from each facility to the simulated monthly average sulfate concentrations. The magnitude of the contribution and range of influence of the emissions is displayed. The region of influence is greatest for emissions from facility #1.

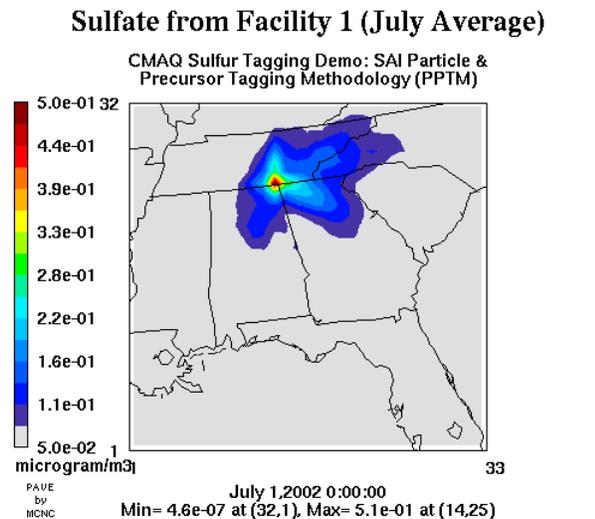


Fig. 1a. Contribution to simulated monthly average sulfate concentration (μgm^{-3}) from example facility #1.

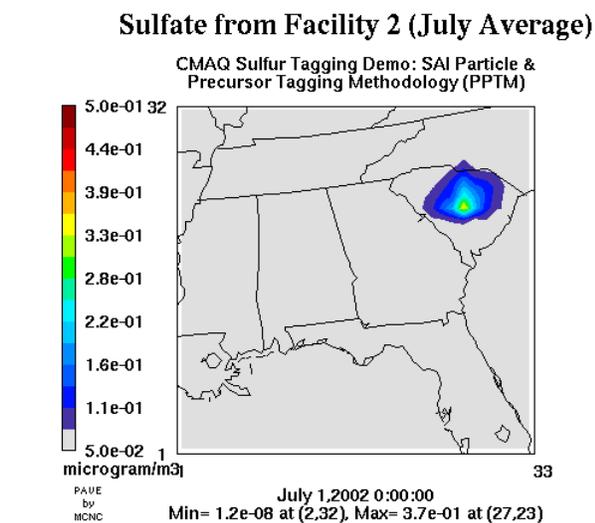


Fig. 1b. Contribution to simulated monthly average sulfate concentration (μgm^{-3}) from example facility #2.

Sulfate from Facility 3 (July Average)

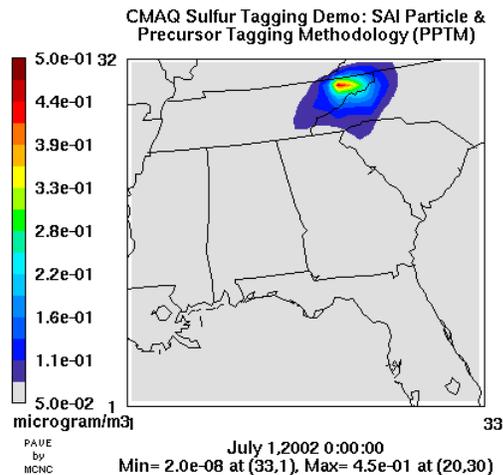


Fig. 1c. Contribution to simulated monthly average sulfate concentration (μgm^{-3}) from example facility #3.

The bar chart in Figure 2 quantifies and compares the contribution from each facility to the simulated monthly average sulfate concentrations at the Great Smoky Mountains National Park IMPROVE site. For this site and time period, the contribution from facility #1 is the greatest.

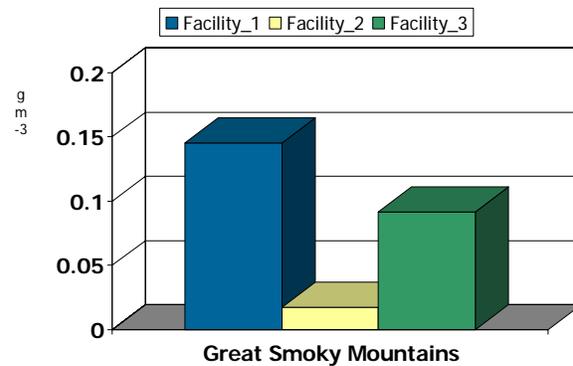


Fig. 2. Contribution to simulated monthly average sulfate concentration (μgm^{-3}) at the GRSM IMPROVE sites from three example facilities.

5. EXAMPLE FOR NITROGEN TAGGING

PPTM for nitrogen has also been incorporated into version 4.5 of CMAQ. Modifications to CMAQ involve several existing subroutines and INCLUDE files, as well as the addition of new subroutines and INCLUDE files. The tagged elements for nitrogen tagging include approximately 14 gaseous and particulate nitrogen species.

The gas-phase chemistry routines have additional production and loss terms added for the tags of NO, NO₂, NO₃, N₂O₅ and these are apportioned based on NO_x totals for each tag. Concentrations for several other nitrogen species tags (e.g., PAN and HNO₃) are calculated with additional chemical rate terms. The production/loss terms for tags are adjusted so that the net production/loss for the sum of tags matches that for the whole.

To illustrate the nitrogen tagging methodology, we tagged the emissions from electric generating units (EGUs) and all other non-EGU point sources in the Southeast and applied CMAQ for a one month period in July 2002. An early version of the VISTAS regional planning organization CMAQ modeling database was used for this example analysis.

The bar chart in Figure 3 quantifies and compares the contribution from each group of sources to the simulated monthly average nitrate concentrations at the Great Smoky Mountains National Park IMPROVE site. For this site and time period, nitrate comprises a relatively small portion of overall PM_{2.5} and the contributions from both EGU and non-EGU point sources is a small portion of the nitrate.

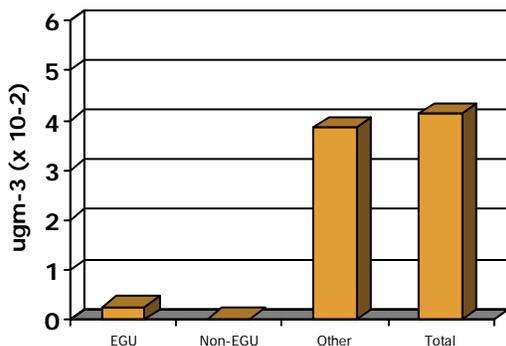


Fig. 3. Contribution to simulated monthly average particulate nitrate concentration (μgm^{-3}) at the GRSM IMPROVE sites EGU and non-EGU point sources.

6. PPTM CPU REQUIREMENTS

CPU requirements will vary according to type and number of tags. We estimate that three sulfur tags will increase the CPU requirements for an average simulation by approximately 50 percent.

Three nitrogen tags will increase the CPU requirements by approximately 80 percent.

7. REFERENCES

CMAS, 2006: User instructions for CMAQ available online at www.cmascenter.org.

Douglas, S., T. Myers, Y. Wei, 2006: *Implementation of Mercury Tagging in the Community Multiscale Air Quality (CMAQ) Model*. Prepared for the U.S. EPA, Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina. Prepared by ICF International, San Rafael, California (06-051).

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SAI, 2005: *User's Guide to the Regional Modeling System for Aerosols and Deposition (REMSAD), Version 8*. Prepared by ICF International, San Rafael, California. Available at www.remsad.com.