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## **Planning for the WRAP Source Apportionment Modeling**

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## Background

Impairment of visibility in Class I areas is caused by a combination of local air pollutants and regional pollutants that are transported long distances. To develop effective visibility improvement strategies the WRAP member states and tribes need to know the relative contributions of local and transported pollutants and which emissions sources are significant contributors to visibility impairment at a given Class I area.

A variety of modeling and data analysis methods can be used to perform source apportionment of the PM observed at a receptor site. Here we focus on methods that employ gridded air quality models. Model sensitivity simulations have been used in which a “base case” model simulation is performed and then a particular source is “zeroed out” of the emissions. The importance of that source is assessed by evaluating the change in pollutants at the receptor site, calculated as pollutant concentration in the sensitivity case minus that in the base case. This approach is known as a “brute force” sensitivity because a separate model simulation is required for each sensitivity.

An alternative approach is to implement a mass tracking algorithm in the air quality model to explicitly track for particular emissions sources the chemical transformations, transport and removal of particulate matter (PM) that was formed from that source. Mass tracking methods have been implemented in both the CMAQ and the CAMx air quality models. Initial work completed by the WRAP Regional Modeling Center during 2004 use the CMAQ Tagged Species Source Apportionment (TSSA) method. There were problems in mass conservation in the version of CMAQ used in that study and this affected the TSSA results.

A similar algorithm has been implemented in CAMx, the Particulate Source Apportionment Technology (PSAT). Comparisons of TSSA and PSAT showed that the results were qualitatively similar, i.e., the relative ranking of the most significant source contributors were similar for the two methods. However, the total mass contributions differed. We are currently implementing a version of TSSA in the new CMAQ release. However this will not be completed until 2006. Thus, the CAMx PSAT source apportionment method is being used at this stage of the WRAP modeling analysis.

## WRAP Source Apportionment Modeling Objectives

- Identify contributions of emissions by source category and visibility-impairing species to modeled air quality for:
  - 2002 “actual” emissions
  - 2000-04 “baseline planning period” emissions, fire normalized
  - 2018 “base case projection period” emissions
  - 2018 “control strategy scenario(s)” emissions
  - Difference plots and tables for the results of these runs
- Prepare results data for the Technical Support System “footprint” maps, charts, and tables
- Execute and report on sensitivity modeling runs to complement the apportionment modeling

## CAMx Particulate Source Apportionment Technology

PSAT performs PM source apportionment for each user defined source group. A source group consists of a combination of a geographic regions and emissions source category. Examples of source regions include States, nonattainment area and counties, whereas examples of source categories include mobile sources, biogenic sources, elevated point sources and even an individual source. The user defines a geographic source region map to specify the source regions. The user then inputs each separate source category as separate gridded low-level emissions and/or elevated point source emissions. The model then determines each source group by overlaying the source categories on the source region map. The Appendix to this document provides a more complete description of the PSAT implementation in CAMx with additional details available in the user's guide (ENVIRON, 2005; www.camx.com).

Source apportionment can be performed for the following PM species in CAMx: sulfate (SO<sub>4</sub>); nitrate (NO<sub>3</sub>) and ammonium (NH<sub>4</sub>); secondary organic aerosols (SOA); elemental carbon (EC); primary organic aerosol (POA); crustal fine; other fine; crustal coarse; and other coarse. The computational cost for each of these species differs because additional tracers must be used to track chemical conversions of precursors to the secondary PM species SO<sub>4</sub>, NO<sub>3</sub>, NH<sub>4</sub> and SOA (See the Appendix). Table 1 summarizes the computer run time required for each of the species. The practical implication of this for WRAP is that it is much more expensive to perform CAMx PSAT simulations for NO<sub>3</sub> and especially SOA then for other species. Computational costs are roughly proportional to the total number of species tracers and emissions source groups used. In each of the benchmark test cases in Table 1 we used 6 emissions category groups and 18 source areas for a total of 108 source groups.

**Table 1.** Benchmarks for PSAT computational costs for each PM species. Run time is for one day (01/02/2002) of the WRAP 36-km domain.

Species	Number of species Tracers	RAM Memory	Disk Storage per day	Run Time with 1 CPU no OMP	Run Time with 2 CPU OMP
SO <sub>4</sub>	2	1.6 GB	1.1 GB	4.7 hr/day	4 hr/day
NO <sub>3</sub>	7	1.7 GB	2.6 GB	13.2 hr/day	Not tested
SO <sub>4</sub> & NO <sub>3</sub> combined	9	1.9 GB	3.3 GB	16.8 hr/day	Not tested
SOA	14	6.8 GB	Not tested	Not tested	Not tested
Primary PM species	6	1.5 GB	3.0 GB	10.8 hr/day	Not tested

The six emissions groups included in the Table 1 benchmarks were:

- Group 1: all stationary sources including offshore
- Group 2: all anthropogenic fire in WRAP region
- Group 3: mobile sources (on road & off road)
- Group 4: all natural emissions including natural fire in the WRAP region and biogenics
- Group 5: elevated fire in other RPOs
- Group 6: everything else: such as wind blown dust, etc

Different groupings of emissions categories can be prepared. For example, if we use PSAT to track SOA sources we would use a different combination of emissions groups that focused more on isolating the VOC species that are precursors to SOA. There is considerable effort and cost in disk storage in preparing the emissions groups, so careful planning is required to avoid excessive or duplicative effort in the emissions processing. The RAM requirement for the SOA benchmark exceeds the capacity of our test machines so we were not able to develop benchmarks for SOA tracers. We can either reduce the number of emissions groups or install additional RAM to complete the SOA benchmarks.

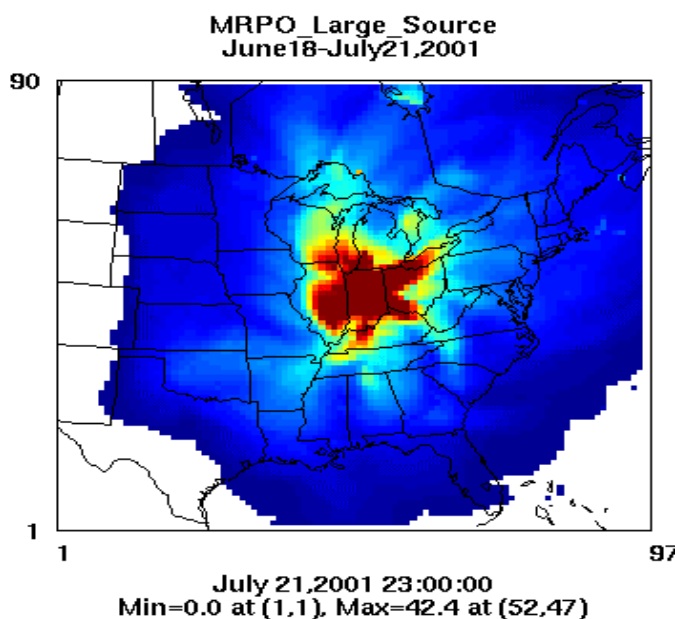
### **Presenting Results of PSAT Analysis**

The source apportionment algorithms implemented in CAMx and CMAQ produce an output file in the same format as the modeled species concentrations. This typically consists of a two-dimensional gridded data set of hourly average surface concentrations for each source group tracer that gives the contribution of the tracer to all the surface grid cells in the model domain for each hour of the simulation. Three-dimensional instantaneous concentrations are also output for the last two hours of the simulation that are used to restart the model. Although there are options to output hourly 3-dimensional hourly average tracer concentrations, because of the vast disk storage needed for the 3-dimensional file we typically save this only for the model surface layer. These model results are typically presented in two different ways:

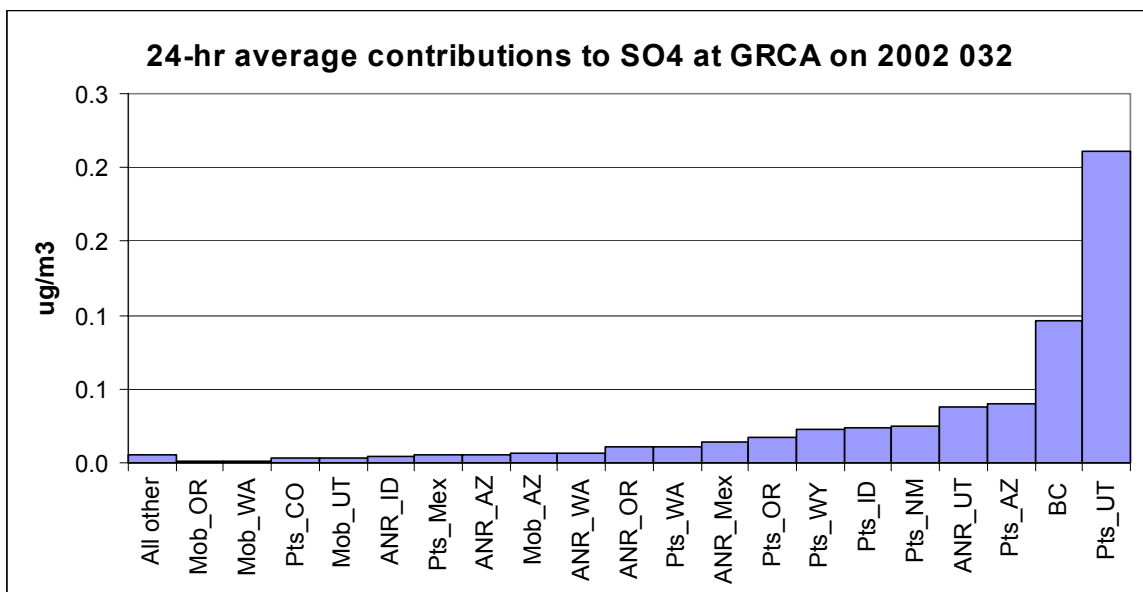
- Spatial plots showing the area of influence of source groups on PM species throughout the model domain, either at a given point in time or averaged over some time interval. Figure 1 provides an example plot.
- Bar plots showing the rank order of source groupings that contribute to PM species at any given receptor site. These can also be at a particular point in time or averaged over selected time intervals, e.g., the average source contributions for the 20% worst days. Figure 2 provides an example plot.

If the 3-dimensional tracer output files are saved it is also possible to prepare animations of PM species plumes from each of the source groups, however, these plots are less useful than the others for quantitative analysis, are expensive to produce and requiring saving 3-dimensional hourly output which is disk space intensive. The primary product of the WRAP PSAT modeling will be bar plots (as in Figure 2) showing the top contributors for the model grid cells containing each IMPROVE site and other receptor sites as identified by WRAP.

**Schedule for WRAP Region PSAT Modeling** We are currently performing PSAT modeling for the 2000-04 “baseline planning period” modeling scenario. We also plan to perform PSAT modeling for the 2018 base case period”, 2018 “control scenario(s)”, and a final 2002 “actual” modeling scenario. It is likely that we will need to complete PSAT runs which complement each routine model run, over the next 12 months.



**Figure 1.** Example spatial display of the PSAT tracer for sulfate from Indiana point source SO<sub>x</sub> emissions averaged for July 18-21, 2002.



**Figure 2.** Source apportionment results at a Grand Canyon (GRCA) IMPROVE receptor site showing the largest source groupings that contributed to the sulfate for the CAMx model simulation February 1, 2002.

## Appendix

# Formulation of the CAMx Particulate Source Apportionment Technology

The CAMx Particulate Source Apportionment Technology (PSAT) is designed to source apportion the following PM species modeled in CAMx:

- Sulfate (SO<sub>4</sub>)
- Particulate nitrate (NO<sub>3</sub>)
- Ammonium (NH<sub>4</sub>)
- Particulate mercury (Hg(p))
- Secondary organic aerosol (SOA)
- Six categories of primary PM
  - Elemental carbon (EC)
  - Primary organic aerosol (POA)
  - Crustal fine
  - Other fine
  - Crustal coarse
  - Other coarse

PSAT performs PM source apportionment for each user defined source group. A source group consists of a combination of a geographic regions and emissions source category. Examples of source regions include States, nonattainment area and counties, whereas examples of source categories include mobile sources, biogenic sources, elevated point sources and even an individual source. The user defines a geographic source region map to specify the source regions. The user then inputs each separate source category as separate gridded low-level emissions and/or elevated point source emissions. The model then determines each source group by overlaying the source categories on the source region map.

The PSAT “reactive tracers” that are added for each source category/region are described below, where subscript (*i*) indicates the number of source groupings. In general, a single tracer can track non-reactive, primary PM species whereas secondary PM species require several tracers to track the relationship between gaseous precursors and the resulting PM. Particulate nitrate and secondary organics are the most complex species to apportion because the emitted precursor gases (NO<sub>x</sub> and VOCs) are several steps removed from the resulting PM species (NO<sub>3</sub> and SOA). The PSAT tracers for each type of PM are listed below. There is a PSAT convention that tracer names for particulate species begin with the letter “P.”

### Sulfur

SO<sub>2*i*</sub> Primary SO<sub>2</sub> emissions

PS<sub>4*i*</sub> Particulate sulfate ion from primary emissions plus secondarily formed sulfate

**Nitrogen**

- RGN<sub>i</sub> Reactive gaseous nitrogen including primary NO<sub>x</sub> (NO + NO<sub>2</sub>) emissions plus nitrate radical (NO<sub>3</sub>), nitrous acid (HONO) and dinitrogen pentoxide (N<sub>2</sub>O<sub>5</sub>).
- TPN<sub>i</sub> Gaseous peroxy acetyl nitrate (PAN) plus peroxy nitric acid (PNA)
- NTR<sub>i</sub> Organic nitrates (RNO<sub>3</sub>)
- HN3<sub>i</sub> Gaseous nitric acid (HNO<sub>3</sub>)
- PN3<sub>i</sub> Particulate nitrate ion from primary emissions plus secondarily formed nitrate
- NH3<sub>i</sub> Gaseous ammonia (NH<sub>3</sub>)
- PN4<sub>i</sub> Particulate ammonium (NH<sub>4</sub>)

**Secondary Organic Aerosol**

- ALK<sub>i</sub> Alkane/Paraffin secondary organic aerosol precursors
- ARO<sub>i</sub> Aromatic (toluene and xylene) secondary organic aerosol precursors
- CRE<sub>i</sub> Cresol secondary organic aerosol precursors
- TRP<sub>i</sub> Biogenic olefin (terpene) secondary organic aerosol precursors
- CG1<sub>i</sub> Condensable gases from toluene and xylene reactions (low volatility)
- CG2<sub>i</sub> Condensable gases from toluene and xylene reactions (high volatility)
- CG3<sub>i</sub> Condensable gases from alkane reactions
- CG4<sub>i</sub> Condensable gases from terpene reactions
- CG5<sub>i</sub> Condensable gases from cresol reactions
- PO1<sub>i</sub> Particulate organic aerosol associated with CG1
- PO2<sub>i</sub> Particulate organic aerosol associated with CG2
- PO3<sub>i</sub> Particulate organic aerosol associated with CG3
- PO4<sub>i</sub> Particulate organic aerosol associated with CG4
- PO5<sub>i</sub> Particulate organic aerosol associated with CG5

**Mercury**

- HG0<sub>i</sub> Elemental Mercury vapor
- HG2<sub>i</sub> Reactive gaseous Mercury vapor
- PHG<sub>i</sub> Particulate Mercury

**Primary Particulate Matter**

- PEC<sub>i</sub> Primary Elemental Carbon
- POA<sub>i</sub> Primary Organic Aerosol
- PFC<sub>i</sub> Fine Crustal PM
- PFN<sub>i</sub> Other Fine Particulate
- PCC<sub>i</sub> Coarse Crustal PM
- PCS<sub>i</sub> Other Coarse Particulate

PSAT includes a total of 32 tracers for each source group (*i*) if source apportionment is applied to all types of PM. Since source apportionment may not always be needed for all species, the PSAT implementation is flexible and allows source apportionment for any or all of the chemical classes in each CAMx simulation (i.e. the SO<sub>4</sub>, NO<sub>3</sub>, NH<sub>4</sub>, SOA, Hg and primary PM classes listed above). For example, source apportionment for sulfate/nitrate/ammonium requires just 9 tracers per source group.

One fundamental assumption in PSAT is that PM should be apportioned to the primary precursor for each type of PM. For example, SO<sub>4</sub> is apportioned to SO<sub>x</sub> emissions, NO<sub>3</sub> is apportioned to NO<sub>x</sub> emissions, NH<sub>4</sub> is apportioned to NH<sub>3</sub> emissions, etc. As a source apportionment method, PSAT must account for all modeled sources of a PM species. Consider two model species A and B that are apportioned by reactive tracers  $a_i$  and  $b_i$ , respectively. Reactive tracers must be included for all sources of A and B including emissions, initial conditions and boundary conditions so that complete source apportionment is obtained, i.e.,  $A = \sum a_i$  and  $B = \sum b_i$ .

The PSAT source apportionment technique has been extensively tested and evaluated against other source apportionment techniques (e.g., ENVIRON, 2005; Morris et al., 2005; Yarwood et al., 2004).

## References

ENVIRON. 2005. "User's Guide – Comprehensive Air-quality Model with extensions, Version 4.20." ENVIRON International Corporation, Novato, California. (Available at <http://www.camx.com>).

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