# USE OF ADVANCED PROBING TOOLS IN ONE-ATMOSPHERE PARTICULATE MATTER PHOTOCHEMICAL GRID MODELS FOR MODEL EVALUATION, CUPLABAILITY ASSESSMENT AND CONTROL STRATEGY DESIGN

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## 1. INTRODUCTION

To address the regulatory requirements of the ozone and particulate matter (PM) air quality standards and the regional haze rule, there is a movement toward using one-atmosphere photochemical grid models that can treat multi-pollutant issues within a common photochemical grid model framework. Such models are quite complex with full–science treatment of many different atmospheric processes (e.g., gas-phase, aqueous-phase and aerosol chemistry; transport and diffusion; wet and dry deposition). Consequently, it is difficult to diagnose why the model obtains the solution it does and identify corrective action when model performance needs improvements or identify the most effective control strategy for reducing concentrations of a desired pollutant.

For ozone modeling, a series of Probing Tools have been developed in the past that help unravel model processes and source-receptor relationships within the photochemical grid model to assist in identifying why the model got the answer it got. These Probing Tools include Process Analysis (PA), the Decoupled Direct Method (DDM) first-order sensitivity approach, and the Ozone Source Apportionment Technology (OSAT). Below we discuss the extension of the Probing Tools to the PM portions of the model and provide examples of the PM Source Apportionment Technology (PSAT) for addressing the requirements of the Regional Haze Rule (RHR).

## 2. EXTENSION OF PROBING TOOLS TO TREAT PM

The three probing tools have been extended to the PM modules in the Comprehensive Air Quality Model with extensions (CAMx; ENVIRON, 2005a). The PM Source Apportionment Technology (PSAT) has been implemented in CAMx for a longer period and has several applications to date. Extension of the PA and DDM to treat PM in CAMx was funded by the Coordinating Research Council under CRC Project A-51a/b and is documented by Koo and co-workers (2006) and are briefly described next.

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## 3. EXTENSION OF PROCESS ANALYSIS TO PM

The CAMx Process Analysis (PA) tools make possible detailed model performance evaluation by tracking the contributions from individual physical and chemical processes governing the fate of the atmospheric pollutants. Using PA, one can more fully understand the complex interactions between the different processes, explain simulation results within the context of the model formulation, and improve the design of control strategies.

CRC Project A-51b has extended the Process Analysis probing tool in CAMx to provide information for the three PM chemistry processes: inorganic aerosol chemistry, organic aerosol chemistry, and aqueous chemistry (Koo et al., 2006). The updated PA implementation was tested and found to be accurate. The existing post-processing tools were also updated for the new PA implementation. The tools produce three bar charts for each species with different degrees of process aggregation to help interpret the process analysis results.

## 4. EXTENSION OF DECOUPLED DIRECT METHOD TO PM

The Decoupled Direct Method (DDM) is an efficient and accurate way of performing sensitivity analysis to model inputs. Traditionally, the brute-force (BF) method has been widely used to study the model responses to various system parameters. While the BF method is easy to apply and interpretation of the result is straightforward, it is computationally demanding and susceptible to numerical uncertainty. The DDM offers an alternative to the traditional brute-force (BF) method by directly solving sensitivity equations derived from the governing equations of the model.

CRC Project A-51a has extended the DDM probing tool in CAMx to include PM chemistry. CAMx PM chemistry consists of three processes: Inorganic aerosol thermodynamics by ISORROPIA, secondary organic aerosol partitioning by SOAP, and aqueous-phase chemistry by RADM-AQ. DDM algorithms were designed and implemented for these three PM modules. Stand-alone model tests for each PM module showed correct implementation and fairly good agreement between the DDM and brute force (BF) methods for 10% input changes.

The completed DDM codes were incorporated into CAMx and tested using a 2-day summer episode for the Eastern US (Koo et al., 2006). In most cases, the DDM first-order sensitivities closely follow those estimated by the BF method. Sensitivities of the organic species involved in SOAP are more linear and agree better between DDM and BF than sensitivities for species involved in ISORROPIA and RADM-AQ (e.g., particulate sulfate, nitrate, ammonium, etc.). Overall DDM performance is in an acceptable range for all species tested.

One of the main advantages of the DDM over the BF method is computational efficiency. As the number of input parameters to which the model sensitivity is calculated increases, the efficiency of calculating the DDM sensitivities becomes higher. When sensitivities are calculated together for 8 input parameters, the DDM is about 1.6 times faster than the BF method.

## 5. PSAT APPLICATION FOR REASONABLE PROGRESS

### *5.1 Regional Haze Modeling*

Five Regional Planning Organizations (RPO) have been formed in the United States to address the requirements of the RHR. One of these requirements is to demonstrate Reasonable Progress by 2018 toward Natural Conditions in 2064 at Class I areas; Class I areas include specific National Parks and Wilderness Areas. The RPOs are using Photochemical Grid Models (PGMs) to project current (2000-2004) visibility to 2018 that is compared to a Uniform Rate of Progress (URP) goal that is obtained by constructing a linear Glide Slope in deciviews from observed current (2000-2004) visibility to Natural Conditions in 2064.

The Central Regional Air Planning Association (CENRAP) is the RPO for the Central States charged for demonstrating Reasonable Progress in visibility improvements at Class I areas. CENRAP has performed preliminary modeling using the CMAQ and CAMx models to project visibility conditions in 2018 for comparisons with the URP goal. Figures 1 and 2 display the modeled 2018 visibility projections and comparisons against the URP goal for, respectively, Caney Creek, Arkansas and Big Bend, Texas Class I areas. The 2018 visibility projections at Caney Creek (22.15 dv) almost achieves (98%) the 2018 URP goal (21.07 dv). However, at the Big Bend Class I area the 2018 visibility projection (16.63 dv) only achieves 20% of the reduction needed to achieve the URP goal (14.73 dv). One potential explanation for why Caney Creek achieves the URP goal whereas Big Bend does not is the due to the higher contributions of International Sources that are assumed to remain unchanged between 2002 and 2018, CENRAP decided to investigate this issue using CAMx PSAT.

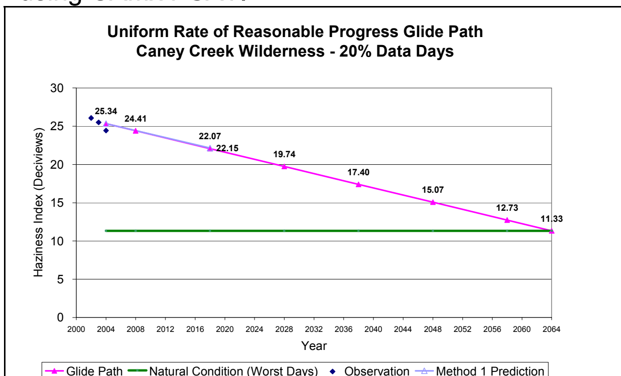


Figure 1. 2018 visibility projections at Caney Creek, Arkansas and comparison with the URP Glide Path goal (CENRAP Base18e2).

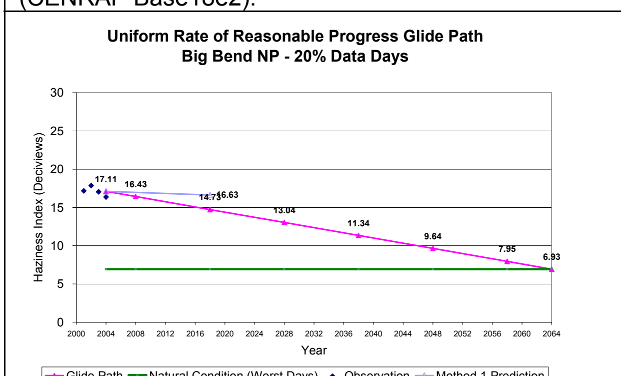


Figure 2. 2018 visibility projections at Big Bend, Texas and comparison with the URP Glide Path goal (CENRAP Base18e2).

### *5.2 Initial CENRAP PM Source Apportionment Modeling*

CENRAP performed a geographic PM Source Apportionment Technology (PSAT) using CAMx and the 2018 Base E emissions scenario. Figure 3 displays the geographic source regions used in the PSAT run that includes separate contributions for each CENRAP State and adjacent States as well as Canada and Mexico. For this PSAT run, only geographic sources apportionment was performed with no stratification by source categories.

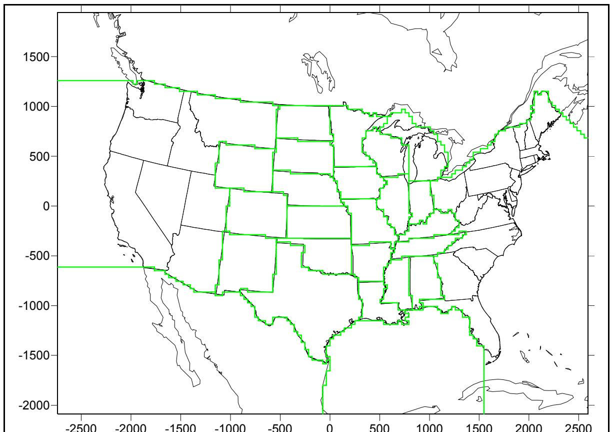

Figure 3. Geographic source regions used in CENRAP initial PSAT PM source apportionment modeling.

### *5.3 Initial PSAT Results*

The CENRAP initial PSAT simulation provided the contribution of SO4, NO3, primary PM (EC, OC, PMF and PMC) from each source region (e.g., State)throughout the modeling domain, including the Class I areas. The PSAT output was processed to obtain the geographic contribution to visibility impairment at the Class I areas. Figure 4 displays the PSAT visibility results for Big Bend National Park on the Texas/Mexico border. The different shadings represent contributions from the different source regions, with the top two stacked bars of grey with vertical lines represent the contributions due to secondary organic aerosol (SOA) from biogenic and anthropogenic VOC emissions (i.e., no geographic source apportionment for SOA). The three largest contributing source regions are Texas (red dots), Mexico (green) and Boundary Conditions (BCs, grey horizontal lines) that contribute, respectively, 23%, 29% and 27% (~80% total) to visibility impairment at Big Bend National Park. In total, approximately 60% of the estimated visibility impairment at Big Bend National Park in 2018 is due to sources that the U.S. can not control, such as Mexico, Global Transport (BCs) and SOA due to biogenic sources. This is in contrast to Caney Creek Arkansas where only approximately 15% of the visibility impairment is due to these controllable sources.

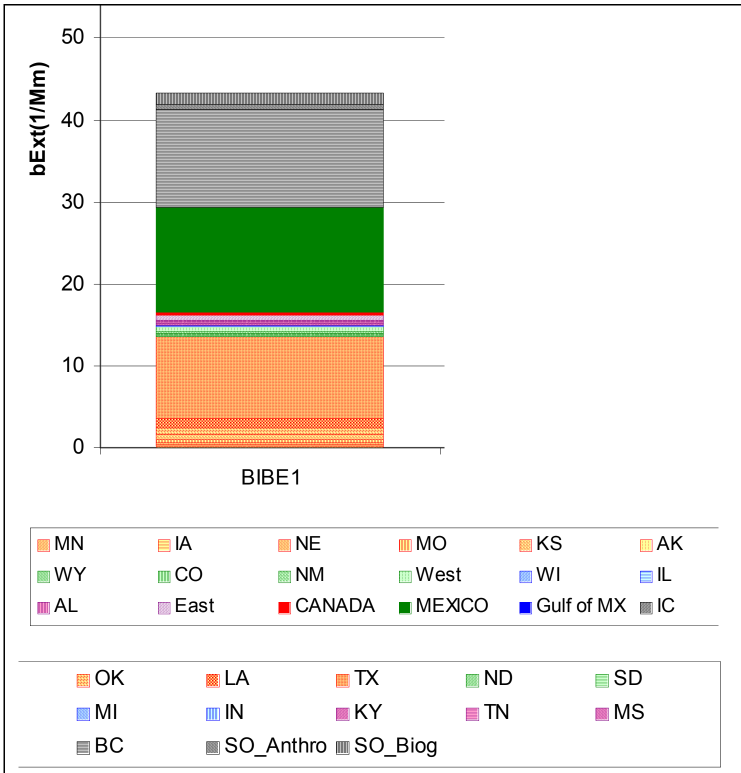

Figure 4. Geographic region contributions to visibility impairment at the Big Bend National Park.

### *5.4 Additional PSAT Modeling*

CENRAP is planning two additional rounds of PSAT modeling. The first round is designed to provide a better estimate of the contribution of anthropogenic U.S. emissions versus uncontrollable sources to visibility impairment at Class I areas. CAMx/PSAT will be run for 2002 and 2018 with separate source regions for U.S. versus international sources and with the emissions split into natural and anthropogenic emission categories. Natural emission source categories would include:

- Biogenic emissions;
- Wildfires; and

- Wind blown dust from natural lands (e.g., not including agricultural lands).

Using these results will allow CENRAP to develop Glide Paths for U.S. anthropogenic sources and account for the contributions of International Transport when determining whether Reasonable Progress is being achieved in 2018.

The second round of PSAT modeling will again separate the modeling domain by States, but provide more detailed assessment of the contributions by source category. More specific, separate PM source apportionment will be obtained by CENRAP State and by:

- Electrical Generating Units (EGUs);
- Non-EGU point sources;
- On-road mobile sources;
- Non-road mobile sources;
- Area sources; and
- Biogenic sources.

The results in the second round of PSAT modeling will be used to assist in the design of control strategies for improving regional haze in the Central States.

## 6. PSAT MODELING FOR SOURCE-SPECIFIC CONTRIBUTIONS

Another element of the RHR is the evaluation of the need for Best Available Retrofit Technology (BART) for specific stationary sources that are shown to contribute significantly to visibility impairment at Class I areas. The Texas Commissions of Environmental Quality (TCEQ) used CAMx and PSAT to perform group exemption modeling of potential BART-eligible sources (ENVIRON, 2005b; Morris and Nopmongcol, 2006). PSAT was configured to work with the full-science Plume-in-Grid (PiG) module in CAMx to better simulate the near-source plume dynamics and chemistry.

The TCEQ BART exemption screening analysis using PSAT/PiG started with the CENRAP annual 2002 36 km modeling database. A 12 km grid was added over Texas and nearby areas as shown in Figure 5. Figure 6 shows the 12 km modeling grid and the locations of potential BART-eligible sources and IMPROVE monitoring sites that include Class I areas. Groups of Texas BART sources were separately modeled using CAMx/PSAT/PiG and the visibility impacts at Class I areas analyzed. Those BART groups whose visibility impacts at Class I areas were below the 0.5 deciview significant threshold were determined to be exempt from the BART process.

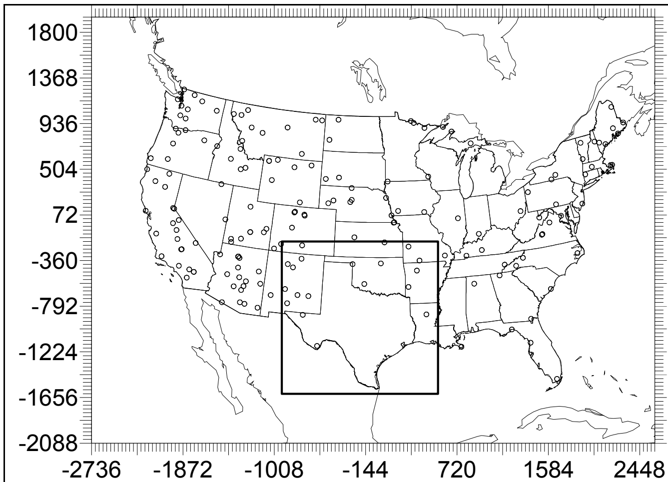


Figure 5. CENRAP 36 km modeling domain with nested 12 km domain for Texas BART exemption screening modeling using CAMx/PSAT/PiG.

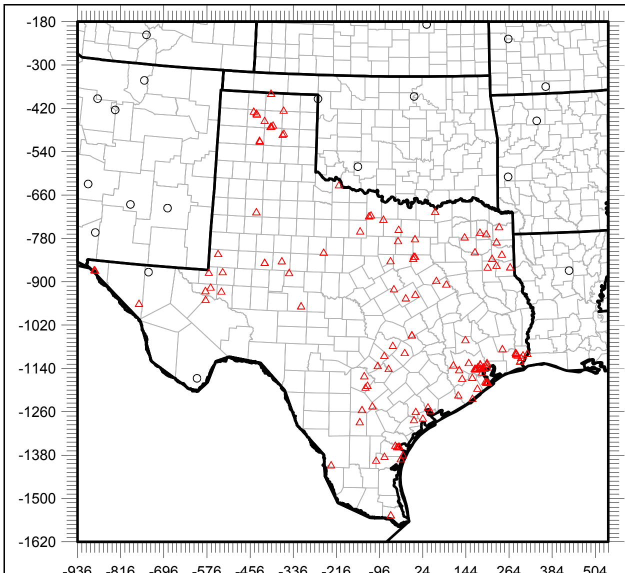


Figure 6. Texas 12 km modeling grid showing potential BART-eligible sources (red triangles) and locations of IMPROVE monitoring sites that include Class I areas.

## 7. CONCLUSIONS

The source apportionment, DDM and PA Probing Tools have been extended to the PM portions of the CAMx model. Preliminary evaluations of the DDM sensitivity approach use for PM has shown in agrees with the Brute Force approach (i.e., two runs, a base and emissions perturbation) for small (10%) changes in emissions (Koo et al., 2006).

The PM Source Apportionment Technology (PSAT) is currently being used by several groups as a diagnostic tool for improving model performance, aiding in the design of control strategies and as a tool for better understanding the contributions to PM and visibility impairment. In additional to CENRAP and Texas, the Western Regional Air Partnership (WRAP) and Midwest Regional Planning Organization (MRPO) have also been using PSAT.

## 7. REFERENCES

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