CMAQ OPERATIONAL EVALUATION OVER THE VISTAS DOMAIN FOR THE 2002 ANNUAL EPISODE

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1.0 INTRODUCTION

The Visibility Improvement State and Tribal Association of the Southeast (VISTAS) is a collaborative effort of state governments, tribal governments, and various federal agencies established to initiate and coordinate activities associated with the management of regional haze, visibility and other air quality issues in the Southeastern United States.

A team of researchers consisting of scientists from ENVIRON International Corporation (ENVIRON), Alpine Geophysics (Alpine) and the University of California at Riverside (UCR) are performing emissions and air quality modeling to assess the effects of future year emission control strategies on visibility and other air quality issues and track reasonable progress toward regional haze goals. Under Phase I, VISTAS modeled January 2002, July 1999, and July 2001 episodes to determine the optional model configuration for EPA's community Multiscale Air Quality (CMAQ) modeling system to be used in annual modeling of 2002 in Phase II.

2.0 OVERVIEW OF THE VISTAS PHASE II MODELING APPROACH

In Phase II VISTAS is performing annual modeling of the 2002 year to develop a modeling database that can be used to project future-year visibility to demonstrate compliance with the regional Haze Rule (RHR) and provide the regional component to demonstrate compliance with the fine particulate ($PM_{2.5}$) and 8-hour ozone standards. The Phase II modeling is being conducted on both a 36 km national US and 12 km grid southeastern US modeling domains. The SMOKE emissions modeling system and the Models-3 CMAQ ozone/PM photochemical grid modeling system were selected as the primary modeling tools for the VISTAS Phase II modeling.

3.0 INITIAL 2002 CMAQ PERFORMANCE EVALUATION

The preliminary evaluation of the initial 2002 CMAQ base case simulation focused on model performance for PM species in the VISTAS states at the IMPROVE, CASTNet, STN, SEARCH and NADP monitoring sites that are shown in Figure 1.

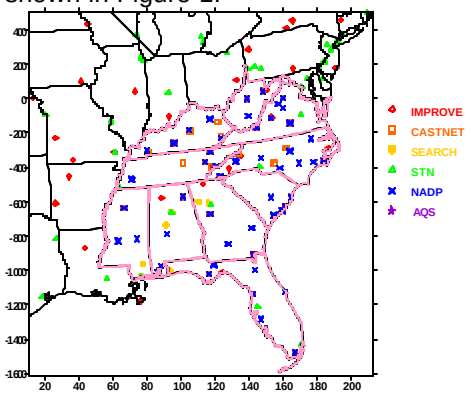

Figure 1. Location of IMPROVE, CASTNet, SEARCH, STN and NADP monitoring sites within the VISTAS States (AQS monitoring site locations not shown due to their sheer number).

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3.1 Model Performance Goals

The issue of model performance goals for PM species is an area of ongoing research and debate. For ozone modeling, EPA has established performance goals for 1-hour ozone normalized mean bias and gross error of #±15% and #35%, respectively (EPA, 1991).

In the VISTAS Phase II initial 2002 CMAQ Base Case modeling, we have adopted model performance goals for bias and gross error as listed in Table 1 that are used to help evaluate model performance. As noted in EPA's draft PM modeling guidance, less abundant PM species should have less stringent performance goals. Accordingly, we are also using performance goals that are a continuous function of average observed concentrations proposed by Dr. James Boylan at the Georgia Department of Natural Resources that have the following features (Boylan, 2004):

- Asymptotically approaching proposed performance goals or criteria when the mean of the observed concentrations are greater than 2.5 ug/m^3.
- Approaching 200% error and "200% bias when the mean of the observed concentrations are extremely small.

Dr. Boylan uses bias/error goals and criteria of ±30%/50% and ±60%/75% and plots bias and error as a function of average observed concentrations. As the mean observed concentration approaches zero the bias performance goal and criteria flare out to ±200% creating a horn shape, hence the name, "Bugle Plots".

Table 1. Model performance goals used in Phase I to help interpret modeling results.

Fractional Bias	Fractional Error	Comment
#"15%	#35%	Ozone model performance goal for which PM model performance would be considered good.
#"50%	#75%	A level of model performance that we would hope each PM species could meet

3.2 Sulfate (SO4) Performance

Sulfate (SO4) is the main contributor to visibility degradation on the 20% Worst days at Class I areas in the VISTAS States. (Brewer, Holman and Hornback, 2003). Consequently, obtaining adequate sulfate model performance is critical for regional haze modeling in the southeastern US.

Figure 2 displays examples of the initial 2002 CMAQ 36/12 km simulation sulfate model performance using the UCR analysis tools. Shown in Figure 2 are scatter plots of predicted and observed sulfate at VISTAS IMPROVE sites during July 2001 and a time series plot for July 2001 at the Great Smokey Mountains National Park. The CMAQ model performance for sulfate and July 2001 is quite good with low bias (< "10%) and fairly low error (<50%). Thousands of these performance plots have been generated an examined. Additional summary performance plots, such as Soccer Plots and Bugle Plots discussed below, are also used.

Soccer Plots are used to display CMAQ sulfate summary model performance across the VISTAS domain by plotting sulfate fractional bias versus error for all networks by season, as shown in Figure 3. Figure 4 displays a time series of sulfate fractional bias across the VISTAS region. These figures provide a summary of the CMAQ monthly and seasonal sulfate model performance across the VISTAS region. The slight winter sulfate under-prediction bias that occurs across all networks but SEARCH is clearly evident in the Soccer Plot (Figure 3, top). During the summer (Figure 3, bottom) the fractional bias is mostly centered on zero and within "15%. The exceptions are the SEARCH Hourly and NADP networks that exhibit a clear overestimation bias. The monthly bias time series (Figure 4) clearly displays the monthly progression of the sulfate bias and summer sulfate overestimation issues at the NADP and SEARCH Hourly networks.

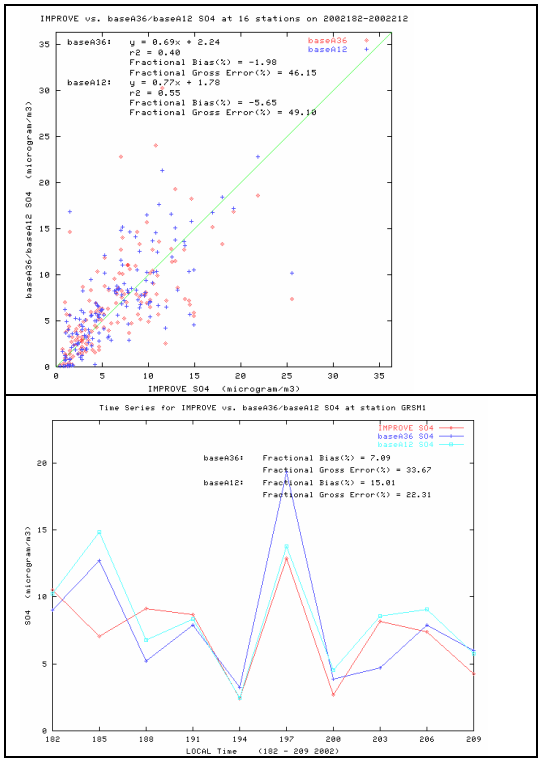

Figure 3. CMAQ 36 km (red) and 12 km (Blue) SO4l performance for July 2001 and IMPROVE sites in the VISTAS States (top) and time series at Great Smokey Mountains National Park (bottom).

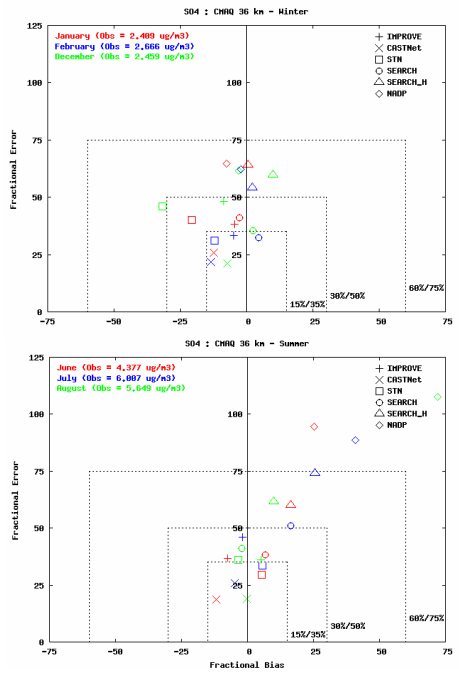

Figure 3. Soccer Plots of CMAQ 36 km sulfate model performance for 2002 displaying fractional bias versus fractional gross error for winter (top), and summer (bottom)

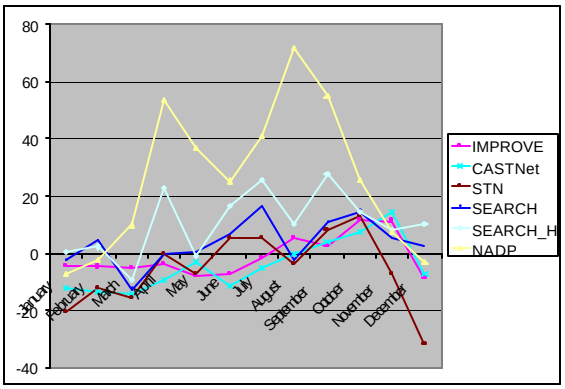

Figure 4. Time Series of SO4 mean fractional bias (%) in the VISTAS States.

3.3 Composite Model Performance Evaluation

The composite model performance of the VISTAS Phase II initial CMAQ 2002 36 km simulation across all PM species using two techniques:

- "Bugle Plots" that compare fractional bias and gross error with performance goals that are a function of average observed concentrations with less stringent performance goals for less abundant species; and
- Visibility performance for the Best and Worst 20% visibility days at IMPROVE sites in the VISTAS region (not shown).

Bugle Plots of Composite Model Performance

Bugle Plots have been developed by Dr. James Boylan of the State of Georgia to account for the magnitude of the concentration to determine whether model performance achieves an adequate level of skill.

Figure 5 displays example Bugle Plots for the initial CMAQ 2002 simulation for all 12 months and the VISTAS region showing the model performance for all PM species across all networks and all 12 months. Sulfate and Elemental Carbon performance is the best followed by ammonium performance. Organic Carbon performance is variable and nitrate performance exhibits an underestimation bias at low observed concentrations (summer) and overestimation bias at higher concentrations (winter). The Bugle Plots indicate that the

summer nitrate fractional bias underestimation is larger than the winter overestimation, yet it is of less importance because of the low observed nitrate concentrations in the summer. The Soil species is overestimated with most of the performance measures falling in the region of poor performance.

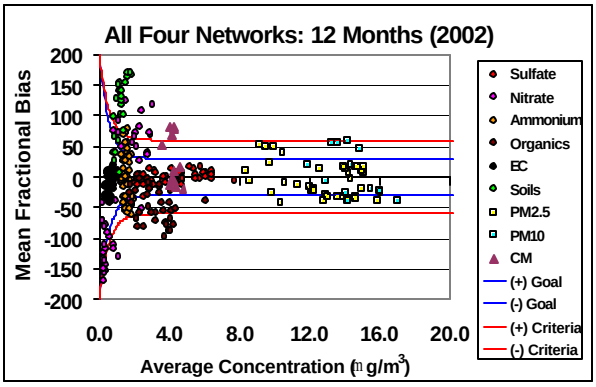

Figure 5. Example Bugle Plots of Mean Fractional Bias for all PM species across all networks).

4.0 CONCLUSIONS

The VISTAS Phase II initial 2002 CMAQ simulation was performed and evaluated using several different analysis tools developed by the VISTAS Modeling Team. The 2002 CMAQ simulation exhibited performance attributes that were generally similar to what was seen in the VISTAS Phase I modeling. Performance for sulfate was by far the best, which is fortunate because sulfate is the most dominant species that contributes to visibility impairment at Class I areas in the VISTAS region on the Worst 20% days. Performance for Elemental Carbon (EC) is next best achieving most performance goals. Nitrate is overestimated in the winter and underestimated in the summer.

Organic Matter (or OC) is underestimated and this is a concern as it is the second most important component of light extinction (after sulfate) in the southeastern US on the Worst 20% days. Soil is generally overstated, especially in the winter and Coarse Matter is also overstated in the winter, but has lower bias in the summer.

The evaluation of the initial CMAQ 2002 Bas Case simulation uncovered some unusual attributes some of which were traced to the emission inputs. For example, an EC overestimation bias at the Everglades IMPROVE site in Southern Florida was traced to errors in airport emissions that will be fixed in the revised CMAQ Base Case simulation

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