Meeting Summary
National RPO Modeling Meeting
May 25 and 26, 2004
Denver, Colorado

Representatives from the Modeling groups for all five of the Regional Planning Organizations met in Denver to discuss their approaches to the modeling work, preliminary results, and future efforts. The final agenda for the meeting and all of the presentations are available at cleanairinfo.com. The meeting included four sessions over a one and a half day period. The first session dealt with *Optimal Model Configuration for PM2.5/Haze Modeling* and the presenters showed results of alternative model configurations. The second session dealt with *Meteorological Modeling.* The third session was a *General Issues and Discussion Session*. The fourth session addressed *Model Performance Issues* and provided an opportunity for interested RPOs to present preliminary results at particular Class I monitor locations to promote discussion regarding consistency, technical approach, and to give an idea how results differ using completely different modeling approaches at such a preliminary stage of the process.

Session I: Optimal Model Configuration - Tuesday 5/25/04 Morning and Afternoon

Fine Grid vs. Coarse Grid Results

Ralph Morris (ENVIRON) spoke on the VISTAS Grid Resolution Sensitivity study. This study compared results for a number of air quality model configurations using the 36 kilometer (km) national RPO grid and the 12 km Southeast U.S. VISTAS grid.

Ralph Morris also gave a presentation entitled "2002 MM5 Model Evaluation: 12 vs. 36 km Results." This study (1) examined the performance of the WRAP configuration of the MM5 model (including Reisner II) using the 36 km grid for 11 subdomains across the nation, (2) compared these results to MM5 modeling using the VISTAS configuration (using Kain-Fritsch [KF] II, Reisner I), and (3) compared results using the WRAP MM5 configuration in four western subdomains for the 12 km and 36 km grids. In discussing the cool, moist bias found in the West, one participant commented that he got similar results in Texas in the BRAVO study (overprediction of convective precipitation using KF), and another noted that VISTAS' results improved when they moved to KF II. The group discussed nudging of the 2-D surface fields, concluding that performance will be improved by nudging only the wind field (instead of all three fields). The group also discussed what effect, if any, collapsing the time steps might have had on the results.

Kirk Baker (Midwest RPO) gave a presentation on Fine Grid Modeling in the Midwest RPO using CAMx4. He noted that the model performance for $PM_{2.5}$ species was very similar for the 36 and 12 km grids. The MRPO has seen some differences between the grids when running control scenarios for nitrate and sulfate, but cannot determine which grid gives more accurate results. The MRPO sized their 12 km grid to include TVA sources and Atlanta. The MRPO made the 12 km grid no larger than necessary because the member states are adamant about performing their own modeling.

Sectional v. Fine/Coarse PM Size Distributions

Gail Tonnesen (University of California, Riverside) discussed Preliminary Results: CMAQ and CMAQ-AIM with SAPRC99; additional analyses are on-going. CMAQ-AIM differs from CMAQ in using a sectional scheme for aerosols with nine sections (instead of a modal scheme), including sea salt chemistry, and using SAPRC99 for gas chemistry. The study gave mixed results, with CMAQ-AIM generally making lower predictions and having a larger negative bias compared to CMAQ. Dr. Tonnesen also discussed an EPRI study that compared CAMx, CMAQ, and CMAQ-MADRID and found that no model clearly outperformed the others. All three overestimated sulfate concentrations and underestimated organic mass. The three models responded very differently to a 50% increase in ammonia emissions, indicating a need to further look at the models' responsiveness to changes in emissions.

Ralph Morris presented Effects of Sectional PM Distribution on PM Modeling in the Western US. He discussed an earlier study in the South Coast Air Basin using CAMx4+, which allows side-by-side comparisons of aqueous-phase chemistry modules (bulk vs. variable size resolution) and of PM size distribution treatments (bimodal vs. sectional). He also presented a WRAP comparison of CMAQ (v4.3), REMSAD (v7), CAMx (bimodal PM), and CAMx (4-section PM).

Initial Boundary Conditions

James Boylan (Georgia DNR) spoke about GEOS-CHEM Modeling for Boundary Conditions and Natural Background. Daniel Jacob at Harvard is running GEOS-CHEM to create temporally and spatially varying boundary conditions for the 36 km national modeling grid for calendar year 2002. All RPOs can use these values, which differ from the EPA default values (sometimes significantly). An interface program will convert the GEOS-CHEM output to CMAQ input. The group discussed a number of potential issues, including (1) inflow/outflow discrepancies between GEOS-CHEM and MM5, (2) the interface of the planned 4°x5° GEOS-CHEM grid with the 36 km grid, (3) incoming ozone over the Pacific, (4) the handling of Asian dust plumes, and (5) a discrepancy between GEOS-CHEM and CMAQ regarding $PM_{2.5}$ and PM_{10}. Mr. Boylan also discussed two potential methods for using GEOS-CHEM to evaluate natural background levels in Class I areas. A number of participants expressed reservations about the accuracy of GEOS-CHEM for this purpose.

Application of Multiple Models

Calvin Ku (Missouri DNR) presented CMAQ and CAMx Simulations for January and July 2002 (basB). He noted that the results were mixed for the models over CENRAP generally. The study also showed mixed results for the models in three climatically different regions in CENRAP that contain Class I areas, with varying performance depending on region and season. This finding points up the difficulty in improving model performance over the whole CENRAP domain. Mr. Ku also noted that CAMx uses less computer resources than CMAQ.

Ralph Morris discussed the Application of Multiple Models to Fine Particulate Simulation in the Southeastern US. Both models performed reasonably well, with CMAQ performing better for SO4 and CAMx performing better for carbon. He noted that CMAQ performance for carbon improved when they adjusted the Kz_min value to 1.0 m^2/sec (from 0.1m^2/sec). He pointed out a number of advantages to running multiple models, and noted that set-up time for running a second model are minimal because there are emissions processors available for converting CMAQ inputs to CAMx format and vice versa. Mr. Morris indicated that they used fractional bias and fractional error (instead of normalized) to illustrate model performance because these statistics do not exhibit such extreme fluctuation.

Ralph Morris also presented WRAP 1996 Multi-Model Evaluation. This study compared CMAQ (v4.3), REMSAD (v7), CAMx (bimodal PM), and CAMx (4-section PM) using the 1996 36 km section 309 database. He noted that SO4 was the best performing species on an annual basis, with a winter overprediction compensating for a summer underprediction; that NO3 was predicted poorly by all models; and that OC, EC, and CM were underpredicted by all models. He concluded that modeling is more challenging in the West than in the Midwest and Southeast.

Chemical mechanisms for PM: CB4, CB4-2002, SAPRC-99

Gail Tonnesen presented Model & Chemistry Intercomparison: CMAQ with CB4, CB4-2002, SAPRC99. She discussed some chemistry differences in the models and presented results for the U.S. and the VISTAS states. The performance of CB4 and CB4-2002 was similar, and superior to SAPRC99 overall (though more diagnostic evaluation is needed). Given that the computational cost of SAPRC99 is twice that of CB4, she recommends using 36 and 12 km grids with CB4 chemistry for the time being. She also advocates looking at model responsiveness to control strategies.

Probing/Apportionment Tools

Gary Kleiman (NESCAUM) discussed REMSAD Version 7.10 with Source Tagging. This exercise (tagging sulfur species emissions by state) was carried out to evaluate the REMSAD tagging technique for MANE-VU, not to look closely at the results. He said the next steps are to develop preliminary state contributions to sulfate from elevated point sources for contribution assessment, do performance evaluation using 2002 meteorology and emissions, and to explore surface emissions tagging and nitrate tagging. The long-range plan is to apportion emissions by state and use the results for SIP development. The group discussed what types of emissions are included in elevated point sources and surface sources.

Gail Tonnesen presented information on Modeling Source Apportionment for the WRAP. She discussed the "tagged species" approach to track mass from a single source. University of California - Riverside and ENVIRON are working to add the tagging algorithms to CMAQ and CAMx. These tracers will allow tracking of emissions from a certain region or source category, producing 3-D plots of concentrations resulting from the tagged emissions and bar charts of the contributions at each receptor site. To determine where emissions of the tagged species result in lower concentrations of secondary species, the concentration results must be compared to the

base case. To trace the contribution of a single source, its emissions must be input as a separate file (i.e., not through SMOKE). They expect to be able to designate around 20 to 40 tracers per run.

Ralph Morris discussed Implementing PM Source Apportionment (PSAT) in CAMx for MRPO. This approach allows up to 36 tracer classes. Results for sulfates show that there is good agreement between PSAT and the zero-out sensitivity analysis. PSAT can potentially be used for diagnostic testing and evaluation, source culpability assessment, and control strategy design.

Modeling Options for BART Assessment

Ralph Morris described four Modeling Options for the Proposed BART Rule (CALPUFF, SCICHEM, CMAQ, and CAMx) and listed the advantages and disadvantages of each. He suggested one potential approach using CAMx/PSAT to address each state one at a time.

Session II: Meteorological and Emissions Modeling - Tuesday 5/25/04 Afternoon

Fire Emissions Modeling

Dave Randall (Air Sciences) presented Process & Method for Developing Model-Ready Files of Emission Inventories for Wildfire, Prescribed Fire & Agricultural Burning. He indicated that the projected fire inventory for 2018 is event-based, with prescribed and agricultural fires projected for a specific location on a specific day. One participant noted that when such a projection is combined with a specific year's meteorology, a fire may occur on an inappropriate day (e.g., a day with heavy rains). Another pointed out that the wind characteristics on a day with a projected fire will have a large effect on how the fire emissions interact with point source emissions. Concerns were raised about the reliability of the modeling. The next step to improve the fire inventory is to use satellite data and burn scars to track location and vegetation types better. Mr. Randall cautioned against comparing base case impacts (including actual fire events) to projected impacts; instead, the inventory should be used to compare control scenarios.

Meteorological Modeling

Zion Wang (University or California, Riverside) presented 2002 MM5 Model Evaluation: 12 and 36 mm Sensitivity Tests for the WRAP. He discussed model runs made with various configurations of MM5 to evaluate which configuration would give the best results in the WRAP states.

Da-Lin Zhang (University of Maryland) presented an Analysis of the MM5 Simulated Surface Fields with Three PBL Schemes over the Eastern US During August 2002 for MANE-VU. The schemes evaluated were Pleim-Xiu, Blackadar, and Blackadar plus a land-surface scheme. Of the PBL schemes tested, the Blackadar performed the best overall with good correspondence to the observed diurnal pattern of wind speed and temperature. The Pleim-Xiu scheme more accurately captures the observed diurnal pattern of humidity.

George Bridgers (North Carolina DAQ) discussed VISTAS Meteorological Modeling 2002 Simulation. Model performance was quite good compared with other modeling exercises, with most variables performing best in the VISTAS region. Their cold bias was the inverse of that discussed previously for the West, occurring in the winter mostly during the day.

Session III: Summary of RPO Technical Approaches & Schedules - Wednesday 5/26/04 Morning

Kirk Baker presented a summary of the MRPO Technical Approach. This year MRPO will transition from 1999 to 2002 based anthropogenic emissions submitted from the states. They are using CAMx4 and still having nitrate and ammonia performance problems. The modeling process is iterative, and they will continually update the models until they run out of time and must revise the SIP. The MRPO has been using 14 vertical layers going up to 6 km, but are considering switching to 16 layers (up to 15 km) to be more consistent with others. Calvin Ku mentioned that CENRAP has had a contractor prepare extensive MOBILE6 inputs which MRPO can also use.

Gary Kleiman presented a summary of the MANE-VU Modeling Plans. They intend to use CMAQ for episode analysis to develop control strategies. For annual runs and source apportionment, they intend to use REMSAD (with tagging) and CALPUFF. The use of multiple models for source apportionment will allow a weight-of-evidence approach for SIP development. In discussion, Carey Jang (US EPA) noted that they are now able to run CMAQ in parallel faster than a single serial application of REMSAD using a four-CPU (supercomputer) system. Mr. Kleiman indicated that MANE-VU would consider CMAQ for the annual runs in light of this information, but would still use REMSAD to some extent for source apportionment because of its tagging capabilities.

Pat Brewer (VISTAS) presented the VISTAS Modeling Overview. VISTAS has completed a Phase I model evaluation and written a modeling protocol. Phase II involves annual regional modeling. VISTAS intends to conduct base year modeling to support both regional haze and $PM_{2.5}$ regulatory requirements, then continue with regional haze modeling for future years and control strategies. (The states will be responsible for $PM_{2.5}$ attainment demonstrations.) They are using a "typical year" approach for EGUs and fires in their emissions inventories so that they can compare 2002 and 2018 using the same assumptions. After evaluating the use of DDM for aerosols sensitivity analyses, they have discontinued that approach (time savings offset by added memory requirements). VISTAS is performing some general sensitivity runs using emissions rollbacks in various sectors and areas with the 2018 initial emissions inventory and will make these analyses available to all the RPOs. They are identifying appropriate episodes for modeling using a classification and regression tree (CART) analysis to characterize the relationship between meteorology, $PM_{2.5}$, and visibility.

Calvin Ku summarized the CENRAP Modeling Workgroup approach. They had a problem in Phase I testing with some negative deposition velocities. They traced it to an older version of MM5 and are now using a newly released version (v3.6.3), which has resulted in significant changes in temperatures, mobile emissions, and the concentration and distribution of

ammonia and sulfates. They are continuing to evaluate CMAQ and CAMx, currently performing sensitivity runs to compare performance. They have developed software to compare modeling results to monitoring data, which is available to all RPOs at no cost.

Tom Moore (WRAP) presented on their Attribution of Haze Project. The WRAP will combine information from all types of analyses to determine the causes of haze in their Class I areas. The project will identify geographic source areas of emissions that contribute to impairment at each Class I area, which will help to target inter-state needs. The project will provide clear summaries for policymakers of the estimated areas and sources of impairment for each Class I area, including the associated uncertainty.

Session IV: Model Performance Issues - Wednesday 5/26/04 Morning

Tom Moore made a presentation on Naming Emissions Scenarios for Regional Haze Air Quality Modeling to start discussion on standardizing terminology for clarity. He discussed five stages of regional haze modeling and associated emissions inventories: (1) Initial 2002 Performance Evaluation, (2) Final 2002 Performance Evaluation Modeling, (3) Baseline Visibility Modeling, (4) 2018 Base Case Modeling, and (5) 2018 Control Strategy Modeling. There was general agreement that the last use of actual emission data would be in the first half of 2005 for Final 2002 Performance Evaluation Modeling. The group discussed the use of "typical year" modeling for the baseline period, since the RPOs will not have 2003 and 2004 emissions inventories in time to use in any of the modeling.

Jeff Underhill (New Hampshire DES) led a Model Performance Zone Discussion. The purpose of the zones would be to target where optimal model performance is needed, for example, in Class I areas in each RPO. The group discussed a number of issues including the basis for creating the zones; the possibility of very different model performance at sites within the same zone; and whether urban, rural, and remote sites in a zone should be considered together or separately. The draft zone map was discussed, with some RPOs offering suggestions and others indicating that they would provide comments later.

James Boylan and Kirk Baker discussed Photochemical Model Performance and Consistency. Mr. Boylan presented a comparison of daily modeling results by MRPO, VISTAS, and MANE-VU for a winter and a summer episode at three IMPROVE sites. In some cases there was good agreement among the models and monitors, in others, a lot of variation (even between the two RPOs running CMAQ). It was noted that where models diverge, they may show a different response to control strategies. The group discussed some reasons that could explain variation, including differing Kz_min values, differences in soil methodologies, differences between CB4 and SAPRC99, and potential differences in emissions inventories. Kirk Baker presented a comparison of hourly modeling results by MRPO and VISTAS for a summer episode at the Pittsburgh super site. In some ways these hourly results are better than daily results–they generally capture the diurnal patterns for most pollutants, although the magnitude is considerably off in some cases. For organic carbon, the discrepancy may be related to the conversion factor used to convert carbon to mass.

James Boylan spoke about PM Model Performance Goals and Criteria. He proposed using mean fractional bias (MFB) and mean fractional error (MFE) as the standard performance metrics. Based on benchmarking with a combination of data from numerous PM modeling studies, he proposed goals (close to best achievable) and criteria (acceptable) for these metrics and showed where the modeling studies fall for the various components of PM. Where these metrics fall for a particular modeling exercise would dictate the level of diagnostic study required. The group discussed a number of potential issues, including (1) adjusting the treatment for visibility (rather than $PM_{2.5}$) by multiplying the mass of each species by its extinction coefficient; (2) whether the proposed goals are too lax; (3) whether different goals and criteria should be set for different species; (4) implications of very low concentrations, which are critical in the West; (5) whether MFE is less intuitively meaningful than normalized error metrics; and (6) whether benchmarking should be done for the entire modeling system (meteorology, emissions inventory, and model).