July 20, 2004

2003 Final Report: WRAP Regional Modeling Center

Contract number:

Prepared for:

Western Regional Air Partnership Modeling Forum
Western Governors' Association

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1. Summary

The Western Regional Air Partnership (WRAP) is a partnership of 13 western states designed to promote cooperation in attaining Clean Air Act goals for improving visibility in Class I Areas. The Western Governors' Association (WGA) is supporting through WRAP a Regional Modeling Center (RMC) that includes a team of scientists from the University of California, ENVIRON Corporation, and the University of North Carolina. WRAP contracted to the RMC in 2001-2002 to develop model scenarios and data bases that were required by Section 309 of the CAA to support SIPs for states that opted to participate in the Section 309 process. In early 2003, WGA extended the RMC contract to complete modeling studies in support of Section 309 SIPs and to begin research and development on models and data sets to support SIPs and TIPs that will be prepared under Section 308 of the CAA. The RMC team works primarily with the WRAP Modeling Forum, however, the RMC also interacts with several other WRAP forums and state and tribe staff, and with other contractors who provide emissions data to the RMC.

This final report is submitted by the RMC to WRAP describing accomplishments and deliverables completed as part of the 2003 work plan. The 2003 RMC work plan was divided into 6 major tasks areas included the following:

1) Project management, computers systems and webpage.
2) Completion of §309 modeling and Technical Support Document (TSD)
3) Development of QA procedures and Model Evaluation tools & datasets
4) Air Quality Model Source Apportionment Capabilities
5) Ammonia Inventory and Improvement to SMOKE emissions processing.
6) Develop and process 2002 meteorological fields, identifying and documenting QA/QC procedures, and model development
7) Air Quality Model Source Apportionment Capabilities

Each of these major task areas were comprised of several subtasks. Activities and deliverables related to each subtask is discussed below and summarized in Tables 2 through 10 of this report. In addition, there were several project activities that were not included in the original 2003 work plan, but which were added to the project with the approval of the WRAP modeling forum during 2003. For example, after a bug was discovered by EPA in the CMAQ meteorology preprocessor the RMC performed additional model evaluation and analyses to determine whether this affected the previous modeling results and conclusions for the Section 309 work. These activities are summarized in Section 9.

The 2003 RMC work plan marked a transition from the modeling activities in support of §309 to the development of datasets and tools for use in §308. In general terms, the RMC was focused on completing tasks associated with the §309 TSD during the first several months of 2003, and began to emphasize model and dataset development tasks associated with §308 planning during the late spring and summer of 2003.

We note that because of delays in acquiring input data or completing model simulations, some of the activities and funding planned for 2003 were carried over into early 2004. Most notably, there were important concerns regarding the MM5 model performance in the 2002 simulations for the southwestern US. Because of these concerns we delayed carrying out the 12-km MM5 simulations and as a result some effort budgeted for 2003 was carried over into 2003 for additional testing and evaluation of MM5. Furthermore, because of concerns about the 36-km and nested 12-km MM5 performance, we have delayed completing the annual 2002 12-km MM5 simulation until additional testing of MM5 is completed. However, preliminary work for processing the 12-km emissions was completed so that the 12-km emissions inventory can be completed expeditiously when the 12-km MM5 results become available.

Significant accomplishments during 2003 included the following:

- Completion of the §309 modeling and TSD
- Major improvements and additions in model evaluation data sets and software
- Development and testing of a source apportionment algorithm in CMAQ
- Initial development of emissions, meteorology and air quality model data sets for calendar year 2002 to be used in Section 308 modeling.
- Expansion of computational resources, testing of new versions of CMAQ, and testing & benchmarking CMAQ on a variety of computational platforms and computer operating systems.

There were two modeling forum workshops held as part of the 2003 work plan. A workshop was held on October 8-9 at Riverside to review progress on the work plan and to discuss the schedule for tasks during 2003. Meeting agenda and presentation for the October meeting are available at the RMC webpage:
www.cert.ucr.edu/aqm/308/meetings/mf_agenda_oct2003.htm

A technical workshop was held in Phoenix, AZ on January 28-29, 2004 and the agenda and presentations for this meeting are also available on the RMC webpage: www.cert.ucr.edu/aqm/308/meetings/Jan_2004_ppt/040128Modeling_Workshop_Agenda.htm

Synergistic Activities

Beginning in June 2003 ENVIRON, UCR and Alpine Geophysics LLC began a collaboration to perform visibility modeling for the VISTAS Regional Planning Organization. Because the VISTAS modeling is based on the same 36-km RPO grid used by the WRAP, there is the potential for synergistic benefits from this collaboration. The primary benefit for WRAP during 2003 was that VISTAS supported efforts at UCR to acquire ambient monitoring data sets for the continental RPO grid, and ENVIRON was able to commit addition staff resources to visibility modeling and model evaluation. Although WRAP provides.

2. Project Management and computer systems administration

Table 1 summarizes the project management activities and deliverables. Project management is distributed between the three Co-Principal Investigators with Gail Tonnesen at UCR responsible for overall project management, Zac Adelman at UNC/CEP coordinating emissions modeling and Ralph Morris at ENVIRON coordinating meteorology modeling.

The project webpage is the primary point of sharing model results with the WRAP and stakeholders, and thus maintenance and updates to the project webpage is key task. Because the WRAP 309 and 308 activities each generated many Terabytes of model output, management of disk storage including archiving or back-ups of key is also a major task.

Development and maintenance of computational resources and disk storage are a critical aspect of the project management. Completing model simulations of emissions, meteorology and visibility modeling for annual periods is computationally demanding and until recently was only feasible on supercomputers. As part of the RMC effort during 2001 the UCR modeling group were the first to develop a Linux version of CMAQ and the first to port the parallel version of CMAQ to Linux. The RMC was also able to optimize the hardware configuration to achieve good parallelization efficiency using inexpensive Gigabit Ethernet while other institutions have struggled with poor efficiency on more expensive Beowulf clusters. These accomplishments have made it possible for the RMC to perform annual visibility simulations using CMAQ on relatively inexpensive Linux clusters.

The RMC also provides users accounts to staff at UNC and ENVIRON so that all modeling activities can be completed on computer systems located at UCR.

During 2003 the RMC continued to efforts to test and optimize CMAQ on Linux operating systems, including the following:

- Purchase and installation of several new RAID5 disk storage systems
- Purchase and testing of 4 dual CPU Opteron computers
- Ported CMAQ to the 64bit platform using the Opteron CPU
- Testing and benchmarking of CMAQ release 4.2.2
- Testing and benchmarking of CMAQ release 4.3
- Continued efforts to optimize SMOKE and CMAQ performance using

Because there are substantial periods in any project during which computing resources are not fully utilized, it is beneficial to share computers among different projects. Total disk storage available is 21 Terabytes (TB). As of December 2003 the total investment in computer equipment at UCR was approximately $280k, of which WRAP has contributed $114k. Table 2 lists the computing resources as of December 2003 available for use at UCR by the RMC.

Table 1. Project Activities and deliverables for project management.

Purpose: This task include project management, meetings and phone calls with project sponsors, computer administration, repairs, maintenance and upgrades.
Activities 1. Biweekly conferences calls, project management, and preparation of reports. 2. Follow-up activities for the Section 309 SIP were performed under this task. 3. Updates to computer operating systems: Upgraded disk storage on a RAID5 disk systems. 4. Ordered 4 dual CPU Opteron machines (funding 80% from NSF, 20% from WRAP), ported CMAQ to the 64 bit OS, and compiled CMAQ benchmarks for several different computing platforms. 5. Concluded that Athlon CPUs are more cost effective for small compute clusters, while Opteron CPUs are more cost effective for larger compute clusters, of 16 CPUs or more.
Deliverables 1. RMC contributions to the Section 309 Technical Support Document. 2. Progress Reports and Final Report. 3. Technical presentations for the October 2003 and January 2004 Modeling forum meetings. 4. Section 309 Project webpage 5. Section 308 Project Webpage 6. Expansion and maintenance of computing resources.
Activities carried over into 2004 The January 28-29 2004 Modeling Forum Technical Workshop and reporting for 2003 were completed in 2004.

Table 2. Computer hardware used for the RMC operations at UCR as of December 2003.

Computing Clusters:
- 24-CPU cluster using Athlon MP2000 CPUs (12 machine)
- 8-CPU cluster using Xeon 2.4GHz CPUs,
- 8-CPU cluster using Opteron 64bit CPUs

Networking/File-servers:
- Two dual CPU rackmount file servers
- One 24 port Netgear Gigabit Ethernet switch
- Two 8 port Netgear Gigabit Ethernet switch

Hot-swappable Disk Storage
- Five 8-bay IDE/SCSI RAID5 hot-swap disk systems (4.3 TB)
- Two 8-bay IDE/SCSI RAID5 hot-swap disk systems (4.4 TB)

Secondary Disk Systems located in Compute nodes:
- Twelve 8x120GB RAID5 systems (770 GB available each, 9.2 TB total)
- Four 4x250 GB systems (690 GB available each, 2.8 TB total)

Desktop/Training Systems:
- Eight dual CPU 1-GHz Pentium-3 machines used for training and for desktop machines for staff.

Data Backup:
- Autoloading DLT Tape system (uses 40 GB tapes)
- Autoloading Super DLT Tape system (uses 110 GB tapes)

Other
- SGI Origin 2000 4-CPU System
- Several notebook and desktop Sun and PC systems for staff use

3. Task Area 2 Activities.

The original RMC work plan for 2003 included a task for completion of the §309 modeling and TSD with a budget of $34,315. During 2003 we redirected some of our effort from the original 2003 work plan to correct and repeat some of the 309 modeling which contained errors in the point source emissions inventory, and to investigate and correct errors in the fire emissions.

In early 2003 we discovered an the error in the point source emissions that was a result of a bug in the SMOKE emissions processing system. We discovered that SMOKE is very sensitive to the conditions under which its modules and libraries are compiled. For example, the SMOKE I/O API libraries must be compiled with the same compiler version that is used in compiling the SMOKE executable. The result of this error was that SMOKE "dropped" most of the point source emissions for the state of Wyoming during the emissions processing. This error was not detected in the internal SMOKE QA procedures because the error occurred after the internal QA checks were completed. As a result of this error, the RMC developed an extensive post SMOKE emissions QA procedure. This consists of a "stand alone" set of programs that are used to sum the SMOKE output files and automatically produce QA plots that are then posted to the project webpage. Additional description of these QA procedures is provided in the "WRAP-RMC Emissions Modeling Support" Final Report for 2003.

In February 2003 when we evaluated the results of base and optimal smoke management emissions strategies we discovered unexpected results in the CMAQ prediction, or example, in some regions the optimal smoke management strategy had higher modeled PM concentrations than did the base smoke management strategy. Subsequent investigation of the CMAQ simulations showed that these results were caused by inconsistencies in the preparation of these two sets of prescribed fire emissions inventories. We then repeated the emissions processing and CMAQ simulations for these scenarios.

As a result of both planned and unplanned follow-up 309 work, the RMC's primary activity during January to June was completing model simulations and analysis in support of Section 309 TSD. Table 4 lists the additional model simulations that were completed.

Table 3. Major Work Topic 1 – Task 309 - Finish §309 modeling and TSD

Purpose: Complete modeling and analysis in support of Section 309 SIPs
Activities Several additional SMOKE and CMAQ simulations were performed to complete the Section 309 analysis. These included the following annual simulations for 1996: 1) 2018 Base Case with no smoke management 2) 2018 Base Case with base smoke management 3) 1996 Base Case with base smoke management 4) BART 5) Milestone/Annex 6) NOx Sensitivity 7) PM Sensitivity 8) Combined NOx and PM increase 9) All control case with optimal smoke management 10) All control case with base smoke management
Deliverables Model data sets available on project website, and selected model results submitted to WRAP. Chapters submitted for Section 309 Technical Support Document (TSD).

Task Area 2 Activities.

Task area 2 activities include Development & Document of quality assurance procedures; development of a version control and case control system for model data sets; diagnostic analyses to better understand the model performance, and development of model analysis/post-processing software.

Quality Assurance Procedures

Development of the new Quality Assurance procedures are documented in the attached 2003 Final Report WRAP-RMC Emissions Modeling Support

Development of Model Evaluation Software

A major effort during 2003 involved the acquisition of "non-standard" ambient data sets and the development of improved software tools and new model performance evaluation metrics for completing model performance evaluations. During the Section 309 activities the RMC relied exclusively on the IMPROVE and CASTNet ambient data for doing model performance evaluations, and UCR developed software for rapidly completing the model performance evaluation using these data sets:

- IMPROVE (The Interagency Monitoring of Protected Visual Environments)
- CASTNET (Clean Air Status and Trend Network)

During 2003 we reviewed the availability of monitoring data from other monitoring networks, and these are summarized in Table 5. We identified the following data sets that would be valuable for use in WRAP model evaluations:

- EPA's AQS (Air Quality System) database
- EPA's STN (Speciation Trends Network)
- NADP (National Atmospheric Deposition Program)
- PAMS (Photochemical Assessment Monitoring Stations)
- PM Supersites.

The original UCR model evaluation package was designed specifically for use with the IMPROVE data and was not well suited for including the new monitoring data sets. Moreover, because of lessons learned in creating and using the original UCR evaluation software we identified a variety of improvements and optimizations for speed, quality assurance and efficiency that were highly desirable. Therefore, UCR redesigned and recoded the evaluation software and also included modules to compare model predictions to the AQS, STN and NADP data sets.

In addition, we modified the evaluation software to compute non-traditional performance metrics as suggested by AER (Christian Seigneur) and EPA (Brian Eder). A major concern in our previous evaluation studies was that the mean normalized error and bias was inappropriate for species with low ambient concentrations. Some 20 different model performance metrics are now included in the package, as described in the documentation for the software evaluation package. (The final documentation deliverable is due in 12/04 but a draft version is available now.) UCR has released the package to a few other institutions for testing. We anticipate providing an Open Source release of the evaluation software to the modeling community in December 2004.

Finally, we evaluated alternative approaches for assessing the spatial variability in the model performance. All evaluation results that we have presented to date employ the use of paired in time and space comparisons of model predictions to ambient measurements. There is the possibility that small errors in wind direction could result in dramatically degraded model performance. This, it is necessary to also evaluate the extent to which the model predictions are mismatched by a few grid cells compared to the data. The best approach that we have identified for performing this analysis is to import ambient data sets into the PAVE vis tool so that spatial variability in the model and ambient data can be evaluated simultaneously, and we developed software to convert the ambient data sets into the PAVE format. Additional research is required to continue to improved methods for performing unpaired in space analysis of model predictions and ambient and data.

Although we invested more effort than anticipated in revising the model evaluation software, the revised package was urgently needed when we began to evaluate the first 2002 CMAQ model results at the end of 2003, and the new ambient data and new performance metrics are essential for the evaluation and interpretation of the model performance.

Diagnostic Evaluation and Process Analysis

During the Section 309 modeling one of the most serious concerns in the CMAQ performance was the large over-predictions of aerosol nitrate, in some cases with a positive bias on the order of 1000%. Bias terms of this magnitude raised important questions about the validity of the CMAQ model. Moreover, CMAQ underwent a series of revisions in by the model developers at EPA in which they implemented different version of the heterogeneous and homogeneous chemical reaction that produce HNO3. When testing an a new CMAQ release in October 2002 UCR found that the large NO3 over-prediction bias had increased from 800% to over 1200%. Therefore, a major emphasis of diagnostic evaluation in 2003 was a evaluation of reactions affecting the formation of nitric acid (HNO3) and aerosol nitrate.

The default Process Analysis (PA) module includes output of key gas phase chemical reactions and the net rate of change in model species from processes such as transport, emissions and deposition. The PA module did not include output for heterogeneous reactions, and therefore we modified the CMAQ aerosol solver to calculate and output the formation of HNO3 from heterogeneous reactions. Because of the approach used in implementing the aerosol solver this required substantial revisions to the CMAQ code to the file output procedures. Our current version of CMAQ automatically creates the PA output file with the heterogeneous HNO3 production rate in all model simulations. We initially implemented this code in CMAQ version 4.2, and then implemented it in each new CMAQ release through CMAQ version 4.3, as discussed below. These outputs were used to provide diagnostic explanations for the changes in the CMAQ model performance for each release. We also experimented with a recently proposed alternative implementation of the heterogeneous HNO3 formation chemistry. Results of this work were presented at the AAAR meeting in San Diego CA on October 22, 2003. (Available on the RMC webpage at: http://pah.cert.ucr.edu/rmc/ppt_files/aaar_2003.ppt)

We also repeated the 1996 base model simulation using new versions of CMAQ including version 4.2.2., version 4.3beta, and version 4.3. Our efforts in redoing the modeling for 1996 was motivated in part by the need to publish this work in the peer reviewed literature and to establish the credibility of the visibility modeling. The results are also expected to benefit the future 309 analysis for the five states opting in to the 309 process. For example, we expect to use the final 1996 model simulation to develop new scaling factors to be use in the relative reduction factor analysis to be used in modeling of progress for the 5 states that have elected to participate in Section 309.

Table 4. Major Work Topic 2 – Tasks 4JKL, 5J, 6 - Develop/Document QA/QC for air quality modeling, Develop version control and case control system for model data sets, Perform diagnostic analyses to better understand the model performance, Model Analysis/Post-processing.

Purpose: Task 4KL: Develop version control system for model data sets. Task 5J: Perform diagnostic analyses to better understand the model performance. Task 6CDE: Develop improved model performance evaluation tools.
Activities **Task 4:** Used concurrent version systems to archive SMOKE input data sets. **Task 5**: Completed using new model performance evaluation tools, evaluation of new CMAQ releases, and UCR revisions to the CMAQ Process Analysis module to include gas phase and heterogeneous HNO3 formation. Repeated 1996 base model simulation using new CMAQ versions: CMAQ version 4.2.2 CMAQ version 4.3beta CMAQ version 4.3 CMAQ version using UCR N2O5 hydrolysis scheme
Deliverables Task 4: Currently using cvs for all SMOKE scripts and input files. Task 4: QA Procedures are documented in the 2003 Emissions Support Final Report. Task 6: Revised source code for model performance evaluation is available by request with plans to release a public, Open Source version in December 2003. Performance evaluation results are available at: http://pah.cert.ucr.edu/rmc/1996/model_performance/model_performance.shtml Technical presentations given at the CMAQ and AAAR meetings are at: http://pah.cert.ucr.edu/rmc/docs.shtml under "Technical Presentations"
Continuing Activities Task 5&6: We are making major revisions to the model performance software to make it more efficient and easier to run. Process emissions for actual 1996 wildfire, Ag and RX, and redo 1996 model simulation. Task 6: Complete roll out of an emissions regression tool for QA on SMOKE output

Table 5. Summary of Ambient Data Monitoring Networks for use in model evaluation.

Monitoring Network	Chemical Species Measured	Sampling Frequency; Duration	Data Availability/Source
The Interagency Monitoring of Protected Visual Environments (**IMPROVE**)	Speciated PM25 and PM10 (see species mappings)	1 in 3 days; 24 hr	http://vista.cira.colostate.edu/improve/Data/IMPROVE/improve_data.htm
Clean Air Status and Trends Network (**CASTNET**)	Speciated PM25, Ozone (see species mappings)	Hourly, Weekly; Hour, Week	http://www.epa.gov/castnet/data.html
National Atmospheric Deposition Program (**NADP**)	Wet deposition (hydrogen (acidity as pH), sulfate, nitrate, ammonium, chloride, and base cations (such as calcium, magnesium, potassium and sodium)), Mercury	Weekly; Week	http://nadp.sws.uiuc.edu/
Aerometric Information Retrieval System (**AIRS**)	CO, NO2, O3, SO2, PM25, PM10, Pb	Varies; Varies	http://www.epa.gov/air/data/
Speciation Trends Network **(STN)**	includes about 215 monitoring stations nationwide	Daily monitoring at about 64 sites	http://www.epa.gov/ttn/
EPA Supersites	Speciated PM25	Varies; Varies	http://www.epa.gov/ttn/amtic/supersites.html
National Park Service Gaseous Pollutant Monitoring Network	Acid deposition (Dry; SO4, NO3, HNO3, NH4, SO2), O3, meteorological data	Hourly; Hour	http://www2.nature.nps.gov/ard/gas/netdata1.htm
Total Ozone Mapping Spectrometer (**TOMS**) - TOMS Aerosol Index	Ozone; Aerosol Index (UV-absorbing particles)	1 Day, Satellite Data	http://toms.gsfc.nasa.gov/eptoms/ep.html

Task Area 3 Activities

As proposed in the work plan, UCR implemented a tagged species source apportionment (TSSA) algorithm in CMAQ version 4.2.2. The algorithm was tested in CMAQ simulations using the WRAP 2002 data sets for January 2002, and results were presented at the RAP Modeling Forum Technical Workshop in January 29, 2004, in Phoenix. The TSSA algorithm was evaluated by comparing the tagged species for particular emissions source categories and source regions to the results of CMAQ sensitivity simulations in which the same source was zeroed out. Although the results of the two methods are not strictly comparable, they are expected to be qualitatively similar, and the test shows that the TSSA algorithm accurately reproduced the shape and direction of the plume that was observed in the sensitivity simulations with the emissions source removed from the model.

Three methods for visualizing the model results were presented at the January Modeling forum meeting:

1. Animation of the surface layer tagged species in PAVE.
2. Animations of the tagged species in 3-d using VIS5D. The RMC developed software to convert the CMAQ files to the VIS5D format for these animations.
3. Bar plots showing the source contributions to particulate species at each receptor site. These plots were produced by a custom software package developed at UCR for this purpose. Because of the large number of model days and receptor sites, it is essential to develop software tools to automate the generations of these bar plots.

We note that since January 2004 we have implemented the TSSA code in CMAQ v4.4, and created an option to avoid creating the 3-d files because they require excessive disk storage and can cause problems with model output when a large number of tagged species are used. A report documenting the source apportionment algorithm and testing is currently under preparation.

Because the source apportionment is a new area of research, we recommend that that results in CMAQ be compared to similar approaches in alternate models such as CAMx. It is possible that problems with mass conservation might affect the algorithm results, and similar results from multiple models would provide increased confidence in the method.

Table 6. Major Work Topic 3 – Task 4I - Air Quality Model Source Apportionment Capabilities

Purpose: Develop algorithms for the CMAQ model to attribute pollutants to source categories in air quality model simulations.
Activities Develop a new source apportionment (Tagged Species Source Apportionment) for use in CMAQ. Implemented and tested the algorithm in CMAQ v4.2.2. Major activities include testing of the algorithm and comparisons with CMAQ sensitivity experiments in which emissions were zeroed for particular source regions and emissions source categories. The change in concentrations in the zero-out sensitivity case relative to the base case are compared to the source apportionment TSSA results to determined whether the results are similar. Additional activities included development of software to display source attributions at receptor sites, and converting CMAQ output files to VIS5D files for 3-d animations. .
Deliverables: Test case and demonstration was presented at the January 2004 modeling forum meeting. Source code in CMAQ v4.2.2 available upon request.
Ongoing Activities Testing and evaluation of the algorithm development of post processing tools to display results at receptor sites is continuing in the 2004 RMC work plan. UCR is also porting the TSSA code to CMAQ v4.4. Recommend that the CMAQ TSSA code be compared with CAMx PSAT to evaluate consistency of results from the two models and methods.

Task Area 4 Activities

Task 4 activities related to emissions processing are described in the attached 2003 Final Report on the Emissions Support Contract.

Activities related to the NH3 emissions model development are described the literature review and technical design document. We expect the NH3 emissions inventory to be completed by July 31, 2004, and a draft final report to be completed by Aug 31, 2004.

The work plan originally called for an NH3 inventory for 1996, but during the course of the NH3 emissions inventory development it became apparent that the inventory would be more useful if prepared for the 2002 modeling. It did not required a significant increase in effort to collect activity data for both 1996 and 2002, therefore the modeling forum approved the recommendation to prepare the inventory for 2002 instead of 1996.

Table 7. Major Work Topic 4 – Tasks 1ACD, 2ABC - Ammonia Inventory Improvement, Temporal Allocation and Chemical Speciation Improvements to the WRAP Point and Area Sources' Inventories, Improve SMOKE Emission Processing System

Purpose: **Task 1A: Develop improved NH3 Inventory** **1CD Temporal Allocation and Chemical Speciation Improvements to the WRAP Point and Area Sources' Inventories** **2ABC Improve SMOKE Emission Processing System**
Activities **Task 1A: NH3 emissions inventory improvements**: Collected activity data for the GIS based ammonia inventory. **Task 1CD and Task 2ABC:** Developed chemical/spatial/temporal allocation process summaries. Developed new chemical/temporal profiles based on review by RMC and WRAP states Updated the QA protocol based on comments received at the WRAP MF meeting at UCR. Presentation at November 4-6, 2003 National RPO meeting in ST. Louis.
Deliverables. Draft QA protocol – see attached 2003 Final Report on the Emissions Support contract. Chemical/temporal profile review worksheets completed and sent to the WRAP states for review. QA protocol presentation for the WRAP RMC meeting created by CEP.
Ongoing Activities Additional deliverables: We expect the emissions NH3 inventory to be complete at the end of July 2004, and a final report shortly thereafter.

Task Area 5 Activities.

Two major components of Task 5 are the preparation of MM5 datasets and emissions inventories for 2002 for the continental 36-km grid and for the nested 12-km grid for the WRAP states.

Development and testing of the MM5 model scenarios is described in the MM5 modeling protocol. As described in the 2003 work plan we anticipated that we would obtain MM5 input data sets and 36 km MM5 output from CENRAP states who were already modeling 2002 and use these data sets in the initial WRAP 2002 36-km modeling, and that we would re-run any MM5 simulations if necessary. Indeed, we obtained MM5 input data sets and scripts from the State of Iowa, and at the October 2003 CMAS meeting we learned that staff at EPA/ORD recommended that the MM5 simulations be run using the Riemann mixed ice scheme. Therefore, instead of using the Iowa 36km grid files that we repeated the MM5 simulations, and used these data sets in the initial 2002 model performance evaluations presented at the January modeling forum meeting. We completed an evaluation of these new MM5 results, and concluded that the MM5 model still failed to meet typical performance benchmarks for meteorology models. Performance was acceptable in most regions of the US, but wind directions bias, humidity and temperature error and bias were unacceptably large. Additional testing of the MM5 at both 36-km and 12-km activities had been planned for the 2003 work plan but were carried over into 2004 and were completed in March 2004. Results of the final report indicate that we still have unacceptably large bias in MM5 simulations, and that additional testing of MM5 is needed. In particular, we ill explore alternative to the Pleim-Xiu land use model and PB scheme, and will investigate other science options. We anticipate these additional testing activities to be completed in the 2004 work plan, and will be completed by December 2004, so that CMAQ modeling in support of the 308 SIPs and TIPs may proceed on schedule.

CMAQ performance results were completed for the summer and winter months using CMAQ v4.3, and these results were presented at the WRAP modeling forum technical workshop in January 2003. The CMAQ model performance evaluation include extensive new ambient data beyond that which was used in the 1996 309 CMAQ performance evaluations.

In general, the CMAQ performance is significantly improved compared to the 1996 modeling. Much of this improvement can be attributed to major updates in the CMAQ model with major new releases of CMAQ by EPA/ORD in July 2002, December 2002, and October 2003. The RMC tested each new release as they became available. The most significant improvements in the model evaluation were for aerosol nitrate and for secondary organic aerosols. It is likely that some of the CMAQ performance improvements resulted from the more accurate emissions inventories and MM5 input data developed for the 2002 modeling. However, further comparison of the 1996 and 2002 CMAQ performance is required to conclusively determine the causes of the improvements in model performance.

Table 8. Major Work Topic 5 – Tasks 2E, 3C, 4DEFH - Process and compare 1996 emissions grown to 2002, Develop and process 2002 meteorological fields, identifying and documenting QA/QC procedures, Air Quality Model Development

Purpose: Develop and test improved and/or alternative model inputs and model formulation. 2E Process and compare 1996 emissions grown to 2002. 3C Develop and process 2002 meteorological fields, identifying and documenting QA/QC procedures. 4DEFH Air Quality Model Development: test PING; nested 12 km grid. 5AGI Revisit 1996 base case model performance with new emissions and model updates 5C Test SAPRC99 chemistry and compare with CB4.(NOTE: We are evaluating an updated CB4 v2002 before completing the SAPRC99 simulations.) 5MN Test REMSAD and CAMx4 and compare with CMAQ
Activities
Deliverables MM5 Modeling Protocol Technical Presentation comparing CMAQ, REMSAD and PMCAMx models.
Activities Carried over into 2004 Begin 12 km 2002 MM5 simulations. Evaluation of revised (mixed ice) 36 km MM5 simulations. Process 1996 36 km MM5 data for input into REMSAD and CAMx4 using the same horizontal Lambert grid and 18 layer vertical layer structure as used by CMAQ. Refine CMAQ-to-REMSAD and CMAQ-to-CAMx emissions, initial concentrations and boundary conditions processors. Modify REMSAD and CAMx4 code to read in three-dimensional coordinates of point source emissions to be consistent with the CMAQ emissions, rather than internal calculation of plume rise as is done in the standard model. Initial testing and evaluation of REMSAD and CAMx4 for January 1996. Run BEIS3 with 36 km MCIP results and compare back to 1996 results Set up SMOKE for processing preliminary 2002 emissions. Implement and test QA system developed by CEP.

Other Project Activities

There were several project activities that were not included in the original 2003 work plan, but which were added to the project with the approval of the WRAP modeling forum during 2003. These are described next.

MCIP Error: In April 2003 EPA staff discovered a bug in CMAQ Meteorology Chemistry Interface Preprocessor (MCIP) that caused the MM5 layers to be incorrectly averaged when collapsing layers from the MM5 output. Because the RMC had used layer collapsing (from the 23 MM5 layers to the 18 layers used in CMAQ) there was a concern as to whether this affected the Section 309 modeling. Therefore, the RMC performed additional model evaluation and analyses to determine whether this affected the previous modeling results and conclusions for the Section 309 work. We performed simulations for the months of January and July to determine the effects of the MCIP error in the WRAP simulations. We found relatively small changes in our base case simulation with the corrected MCIP version 2.1 compared to the original MCIP 2.0.

Vertical Layer Averaging Comparison: We then repeated the vertical layer averaging comparison using the corrected MCIP. Simulations were performed for January and July for models with 8, 12, 18 and 23 layers. In the previous evaluation we focused primarily on O3 and sulfate. In the new evaluation we evaluated other model species and total PM2.5. We noted that even at 18 layers there were relatively large changes in PM2.5 in the 18 layer model compared to the reference 23 layer model. We performed additional layer sensitivity experiment using the VISTAS episodic modeling for January 2002 (in which we averaged from 32 MM5 layers to 19 CMAQ layers) that also confirmed this result.

Although there appear to be relatively large differences in the model results with and without layer averaging, when we compared both types of model simulations to ambient monitoring data we found that the differences between the two model versions were generally much smaller than the differences between the model and the ambient data. Thus, it appears that the layer collapsing does not substantially alter the objective model performance, and we decided to continue with the layer averaging scheme. We concluded that the additional computational cost of using 1:1 mapping of MM5 to CMAQ layers would be prohibitive for the development and testing of the 2002 annual data sets. However, the effects of layer averaging continue to be of concern and we recommend that they be further evaluated. Two possibilities for additional testing include:

- perform a MM5 simulation with fewer vertical layer to determining whether MCIP layer averaging has a larger effect than simply using fewer MM5 layers.

- Perform model simulations for two emissions reduction scenarios: one with the model base case and emissions reduction case using both using a 1:1 mapping of MM5 to CMAQ; and a second case using layer averaging for both scenarios. The model response can then be analyzed to determine if the effect of the layer change is smaller for the "delta" in the sensitivity case compared to the error in the base case. In other words, if the error is consistent across all layer averaged simulations, the use of layer averaging might have little effect on the emissions reduction scenario results.

Because layer averaging is widely used in the air quality modeling community but has not been rigorously evaluated, we recommend that additional work be completed by WRAP or other agencies to evaluate the possible effects of this practice.