

June, 2003 Progress Report
WRAP Regional Modeling Center

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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 interim progress report is submitted by the RMC to WRAP. It describes progress during January-June, 2003. The contract calls for monthly progress reports, however, due to delays in completing the contract and because of additional effort required to revise, correct and complete work for Section 309 deadlines, the January-June activities are being combined in a single progress report. Beginning in July 2003 we will submit monthly project reports as called for in the contract.

The CAA requirements for analysis of visibility are unique among air pollutants because it requires evaluation of a large number of both clean and polluted days. In effect, this requires the performance of annual modeling simulations. In contrast, traditional modeling studies for ozone (O₃) and other pollutants require episodic modeling for a period of a few days or weeks. Moreover, preparation of visibility SIPs require large scale modeling on semi-continental domains. Performing annual modeling simulations for these large domains continues to be resource intensive and challenging in the accurate preparation of model inputs. In January-May of 2003 we discovered errors or other problems in some input data sets, and this required us to repeat some of the modeling analyses that had been completed in 2002. Notable errors included problems in emissions processing that resulted in lost point source emissions in Wyoming, and errors in fire emissions data sets that required us to investigate and repeat several model simulations designed to evaluate fire smoke management strategies. As a result of these problems, we have diverted some of our effort from the original 2003 work plan to correct and repeat the 309 modeling which contained errors in the point source emissions inventory, and to investigate and correct errors in the fire emissions.

Moreover, several delays in processing the WGA contract to UCR and UCR subcontracts to UNC and ENVIRON resulted in additional delays. Currently, all contracts are in place, and UNC began work on the RMC in early July, 2003. ENVIRON has also been delayed in beginning work on the NH₃ emissions model due to delays in executing the subcontract. However, ENVIRON has work continuously on the analysis of the 309

simulations and preparation of the TSD. An UCR sub-contract to ENVIRON was completed early June 2003, and work in the NH₃ emissions model and other 2003 activities is now underway.

Although we are currently behind schedule on the 2003 work plan, there are several important synergies that may allow us to regain some lost time on the RMC project. Both UCR and ENVIRON are also members of the contractor teams for the VISTAS and CENRAP visibility modeling, and ENVIRON is the lead contractor for VISTAS modeling. Activities carried out on these projects should benefit WRAP and should help us to expeditiously complete the RMC objectives for 2003.

The tables below summarize the status on each of the WRAP RMC 2003 major task areas identified in the 2003 work plan.

Modeling of PM and visibility is still very much in a research and development phase with updates or corrections in models and new science information becoming available on a routine basis. Thus, there is some benefit if we are able to adapt the work plan as new information becomes available. Before making changes in the work plan we will consult with and obtain approval from WRAP. Several items of special interest and which may affect the work plan include the recent discovery of a bug in the MCIP preprocessor, the release of CMAQ v 4.2.2, and the availability of an updated version of the CB4 mechanisms. These are discussed next.

MCIP Error: In April 2003 EPA discovered a bug in the MCIP version 1.0 preprocessor which caused errors when MCIP is used to average MM5 layers for the purpose of reducing the number of layers in CMAQ. In 2001 and 2002 the RMC had used layer averaging to reduce the 23 MM5 layers to 18 CMAQ layers. It is likely that this comparison was affected by the MCIP bug. Thus, we have performed a new analysis of MCIP layer averaging using a corrected MCIP v2.1 with simulations for the month of January and July to determine the effects of the MCIP error in the WRAP simulations. Simulations were performed for January and July for CMAQ with 8, 12, 18 and 23 layers. In the previous evaluation we focused primarily on O₃ and sulfate. In the new evaluation we have noted that even at 18 layers there are relatively large changes in PM_{2.5} in the 18 layer model compared to the reference 23 layer model. We plan to perform additional layer sensitivity experiment for VISTAS to confirm this result. We believe that it would be useful to perform a MM5 simulation with fewer vertical layer to determine whether MCIP layer averaging has a larger effect than simply using fewer MM5 layers. We should also perform a BART simulation with 23 layers 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. That is, if the error is consistent across all 18 layer simulations, there may not be much effect on the sensitivity results from using layer averaging.

We also investigated the effect of the updates in MCIP for CMAQ model simulations using the full 23 MM5 layers. We found relatively small changes in our base case simulation with the corrected MCIP2.1 compared to the original MCIP 2.0.

CMAQ Development: We have added an update to the CB4 mechanism (CB4-2002) to CMAQ. It is currently implemented for the GEAR and QSSA solvers, and we are working on the Hertel/MEBI solver. Because the CB4-2002 has much of the updated kinetics data used in SAPRC99, and because CB4-2002 can readily be performed using the existing CB4 emissions files (whereas reprocessing of emissions will be required for SAPRC99) we believe that it would be useful to test the updated CB4 chemistry before doing the SAPRC99 simulations. This is proposed in the work plan is proposed in Table 6 below.

Other notable activities include the following:

Emissions QA: We have continued to do various QA analysis on emissions inventories, including preparing counties totals of emissions, and preparing an emissions QA checklist/protocol.

Model Evaluation: We have modified our model performance software to include several new metrics that have been proposed by EPA and by Christian Seigneur. We plan to redo the 1996 model simulation with all available updates and bug fixes, and use this as a test case for the new performance criteria. We have prepared emissions and MCIP files and plan to complete the revised CMAQ simulation and evaluation by end of July, 2003.

Conclusions

We are approximately 3 to 4 months behind schedule on certain tasks because of the increased effort needed to identify and correct errors in Section 309 emissions and to redo some of the Section 309 simulations. Delays in processing the contracts and sub-contracts for 2003 have also caused us to be behind schedule. We hope to make up some lost time because of synergies in VISTAS and CENRAP projects, and we expect to complete most project tasks by the end of 2003. However, the availability of emissions inputs remains a major uncertainty in starting annual modeling for the year 2002. We plan to redo the CMAQ model performance evaluation for 1996 using updated emissions and models. This should be completed by mid August 2003. Then, we plan to perform a fist iteration of the 2002 modeling using 2002 emissions where available, and using “grown” 1996 emissions if 2002 emissions are not available. This simulation would represent a exercise in debugging the model, emissions and evaluation procedures. We expect that a final 2002 model performance evaluation case will be completed in 2004.

Table 1. Major Work Topic 0 – Project Management, Computer systems administration and maintenance

<p>Purpose: This task include project management, meetings and phone calls with project sponsor, computer administration, repairs, maintenance and upgrades.</p>
<p>Jan-June Activities Biweekly conferences calls, travel to WRAP meetings, preparation of reports. Updates to computer operating systems, installed new disk storage, data backups, maintenance of website etc.</p>
<p>Jan-June Deliverables None</p>
<p>Activities Planned for July Biweekly conferences calls, travel to WRAP meetings, preparation of reports. Computer systems upgrades and maintenance, updates to computer operating systems, data backups, maintenance of website. Testing and benchmarks on new AMD 64 bit Opteron CPUs.</p>

Table 2. Major Work Topic 1 – Task 309 - Finish §309 modeling and TSD

<p>Purpose: Complete modeling and analysis in support of Section 309 SIPs</p>
<p>Jan-June Activities</p> <p>Our primary activity during January to June was completing model simulations and analysis in support of Section 309. Several of the section 309 annual model simulations were corrected and repeated, and several new annual model simulations were performed with different permutations of the emissions inventories. These simulation were designed to correct errors in the emissions of major point sources that primarily affected Wyoming, and to diagnose and correct errors in the fire emissions. Annual simulations that were repeated include the following:</p> <ul style="list-style-type: none"> • 2018 Base Case with no smoke management • 2018 Base Case with base smoke management • 1996 Base Case with base smoke management • BART • Milestone/Annex • NOx Sensitivity • PM Sensitivity • Combined NOx and PM increase • All control case with optimal smoke management • All control case with
<p>Jan-June Deliverables</p> <p>Model data sets available on project website, and selected model results submitted to WRAP. Chapters submitted for Technical Support Document (TSD)</p>
<p>Activities Planned for July</p> <p>Review and edits to TSD as needed. Continue to place model results and QA on project website, as needed.</p>

Table 3. 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.

Jan-June Activities

Task 4: Recommend to use cvs (concurrent version system) for version control of data sets.

Task 5: Deferred until completing new model simulations.

Task 6:

We have complete revised the source code for doing model performance evaluations, made the code more efficient and more readable for future revisions.

We have modified the evaluation software to compute non-traditional performance metrics as suggested by AER (Christian Seigneur) and EPA (Brian Eder), for example, using mean fractional bias.

Have acquired several ambient data sets for 1996 and 2002.

Jan-June Deliverables

Task 6: Revised source code for model performance evaluation is available on the project website.

Activities Planned for July

Task 4: Investigate utility of cvs for large binary data sets.

Task 6: Continuing to acquire ambient data and revise evaluation programs and preprocessing this data for input to model evaluation software..

Table 4. 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.

Jan-June Activities

UCR has developed a tagged species source apportionment (TSSA) algorithm for use in the CMAQ model. Major activities include:

- Modifying CMAQ to read emissions from multiple input files thereby allowing contributions to be evaluated from different source categories (area, mobile, point, Biogenic, fire) .
- Implementing and testing the TSSA algorithm in CMAQ for nitrogen species.

Jan-June Deliverables:

Deliverable date is December 2003, however, preliminary results will be presented at the October modeling forum meeting.

Activities Planned for July

Implementing the TSSA algorithm for aerosol nitrate species.

Evaluating the algorithm in comparison with mobile source sensitivity simulations.

Table 5. 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

Jan-June Activities

Task 1A: NH₃ emissions inventory improvements: a literature review is near completion; UCR/ENVIRON are preparing a detailed work plan and revised schedule which will be ready for review end of July. We have also begun to identify and collect data needed for NH₃ inventories. Identification of available data sources is necessary to determine the approach to used in modeling some components of the NH₃ inventory and in determining the schedule.

Task 1CD and Task 2ABC: No activity, Work will start with UNC sub-contract in place in July, 2003.

Jan-June Deliverables

None

Activities Planned for July

Begin work on Tasks 1CD and Task 2ABC.

Complete literature review and detailed work plan for Task 1A.

Table 6. 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

<p>Purpose: Develop and test improved and/or alternative model inputs and model formulation.</p> <p>2E Process and compare 1996 emissions grown to 2002.</p> <p>3C Develop and process 2002 meteorological fields, identifying and documenting QA/QC procedures.</p> <p>4DEFH Air Quality Model Development: test PING; nested 12 km grid.</p> <p>5AGI Revisit 1996 base case model performance with new emissions and model updates</p> <p>5C Test SAPRC99 chemistry and compare with CB4. (NOTE: We propose to evaluate an updated CB4 v2002 before completing the SAPRC99 simulations.)</p> <p>5MN Test REMSAD and CAMxv4 and compare with CMAQ</p>
<p>Jan-June Activities</p> <p>Acquired MM5 inputs for 2002.</p> <p>Obtained MM5 2002 annual simulation results from Iowa.</p> <p>Implemented an updated version of CB4 in CMAQ (CB4-2002, Jeffries et al., 2002)</p>
<p>Jan-June Deliverables</p> <p>None</p>
<p>Activities Planned for July</p> <p>Select 12 km WRAP domain.</p> <p>Start 36 and 12 km simulations.</p> <p>Complete a new CMAQ 1996 base case performance evaluation with all available updates and corrections to emissions, using the new MCIP v2.2 and CMAQ v4.2.2.</p> <p>Complete test simulations for January/July using CB4-2002 in the new 1996 base case. The CB4-2002 has much of the updated kinetics included in SAPRC99, however, it has less complete organic chemistry which may limit its ability to simulate SOA formation.</p>