Attachment A
Scope of Work

The Contractor will complete the following tasks:

- Task 1: Set up, run, and assess REMSAD for 1996 using 1996 MM5 meteorological fields
- Task 2: Set up, run, and assess Models-3/CMAQ for January and July, 1996 using 1996 MM5 meteorological fields
- Task 3: Provide technical guidance to the WRAP Regional Modeling Center and transfer all relevant files, programs, and documentation to the WRAP
- Task 4: Reporting and communication

The Contractor shall be allowed to apportion the work among itself and the subcontractors as follows:

Task 1:	ENVIRON will be primarily responsible for the REMSAD runs and analysis. MCNC will prepare the emissions inputs. Both MCNC and ENVIRON will participate in analysis of both models (Subtasks 1.5, 1.8, 1.11), with ENVIRON taking the lead. WESTAR will provide expertise about the specific local needs for SIPs and TIPs for the Western states and tribes.
Task 2:	MCNC will be primarily responsible for all aspects of the task. Both MCNC and ENVIRON will participate in analysis of both models (Subtasks 2.5, and 2.8), with MCNC taking the lead. WESTAR will provide expertise about the specific local needs for SIPs and TIPs for the Western states and tribes.
Tasks 3 & 4:	Both MCNC and ENVIRON will document their pieces as part of each subtask, and MCNC and ENVIRON will participate in communication and technology transfer. MCNC will have primary responsibility for the final documentation and communication with the WRAP Modeling Forum and RMC.

The Contractor will use its Data Migration Facility (DMF) to archive all model inputs, outputs, and system configuration information from both ENVIRON and MCNC. Data will be stored in this way for Tasks 1, 2, and 3.

TASK 1: Set up, run, and assess REMSAD for 1996 using 1996 MM5 meteorological fields

Discussion: The subtasks described in this section all work toward providing credible annual REMSAD simulations for a 1996 base case, future year, and control strategy. The analyses from Task 1 are relevant to development of the Section 309 SIPs and TIPs due in 2003. REMSAD is currently in a state of flux, and it cannot be determined at this time which version will be available for this study. Fortunately, with the exception of the extra emissions and initial conditions and boundary conditions (IC/BC) requirements of the SOA module, the basic inputs for REMSAD are identical for the various versions. Accounting for SOA is critical for modeling visibility in the Western states. Thus, the Contractor will develop REMSAD inputs that include all of the data needed for simulation of SOA, as well as the other primary and secondary PM species.

Subtask 1.1: Develop REMSAD modeling protocol

Lead: ENVIRON

In this subtask, the Contractor will develop a REMSAD modeling protocol. This work will be coordinated with Subtask 2.1 to ensure consistent modeling protocols for both REMSAD and CMAQ, to the extent possible. To best

accomplish this subtask, the Contractor will first prepare a draft modeling protocol for review and comments by the WRAP Modeling Forum. Upon receipt of comments, the Contractor will revise the draft document to incorporate them and then submit the final REMSAD modeling protocol.

In preparing the modeling protocol, the Contractor will consider the issues described in Section **Error! Reference source not found.**. In summary, the REMSAD modeling protocol will be a map for ensuring that the Contractor provides analyses relevant to the development of Section 309 SIPs and TIPs, due in 2003. WESTAR will facilitate modeling protocol development by communicating with the states and tribes and ensuring that the rest of the team is fully aware of the local issues of concern. The modeling protocol will describe in detail how the 1996 hourly 36-km REMSAD inputs will be developed, including meteorology, emissions, and ancillary inputs. It will also describe the procedures to be followed in conducting the REMSAD model performance evaluation. In addition, the modeling protocol will outline and describe the approach and procedures to be used in order to assess the visibility changes between the base-year (1996) and the future-year (2018) simulations at each Class I area under consideration. Particular emphasis will be given to the 16 GCVTC Class I areas with respect to visibility impairment.

The deliverables for this subtask will be a draft and final REMSAD modeling protocol submitted to the WRAP Modeling Forum and the RMC. The REMSAD modeling protocol will be included in the Task 1 final report.

Subtask 1.2: Acquire and process 1996 MM5 runs for input into REMSAD

Lead: ENVIRON

For this subtask, the Contractor will process the national 1996 36-km MM5 model output data for input to REMSAD (note that both MCNC and ENVIRON already possess the 1996 MM5 database). The important issues to address are the vertical layer structure, horizontal grid resolution and extent (including extracting the needed region from the MM5 outputs), temporal resolution needed by the REMSAD data files, and quality assurance of the results.

To convert the MM5 output to REMSAD inputs, the Contractor will use software developed by ENVIRON. This software provides a means for format conversion, layer aggregation, grid adjustments from Lambert to latitude-longitude, horizontal spatial aggregation, "windowing" to the smaller Western domain from the national domain, and generation of statistical and graphical analyses used primarily for quality assurance. The Contractor will use some or all of this software to generate the REMSAD input files and to quality assure the results.

ENVIRON already has available the 1996 MM5 model output and all of the non-emission inputs required by REMSAD for the continental U.S. domain at both 56-km and 36-km horizontal resolution with 8 vertical layers as well as 36-km horizontal resolution inputs with 12 vertical layers.

In addition, the REMSAD latitude-longitude input meteorology files need to be converted for input to SMOKE. This will require ENVIRON to develop a REMSAD input-to-SMOKE interface to provide SMOKE the temperature and solar radiation information needed for biogenic and mobile sources.

Deliverables under this subtask will be (1) 1996 annual REMSAD model-ready hourly meteorological input data, (2) documentation of the results and methods, including a limited set of statistical and graphical summaries used for quality assurance, (3) sample UNIX job scripts used in each stage of the processing, and (4) SMOKE-ready meteorological input files on a lat-lon grid for 1996.

Subtask 1.3: Process 1996 WRAP emissions through SMOKE to generate REMSAD model-ready inputs

Lead: MCNC

The purpose of this subtask is to provide suitable REMSAD emissions inputs for an annual 1996 REMSAD model run. To accomplish this, the Contractor will take the following steps: (1) obtain the 1996 WRAP inventory from the WRAP inventory contractors; (2) convert the inventory format if it is not in SMOKE input format; (3) prepare the SMOKE ancillary input files, including spatial surrogates and cross reference files, biogenic land use, temporal profiles and cross reference files, and speciation profiles for REMSAD and cross reference files; (4) configure SMOKE annual run scripts for the Western domain; (5) run SMOKE for all days in 1996 to create the layer-1 and elevated emission input files; (6) quality assure SMOKE outputs, correct inputs, and rerun as necessary; and

(7) document all processing steps and provide an interim report on the emission inputs for REMSAD, suitable for the Task 1 final report (Subtask 1.12).

The Contractor has previously and recently run SMOKE for all days in 1996 for input to CMAQ for a national 36-km domain. This work used the National Emissions Trends (NET) Inventory, now called the National Emissions Inventory (NEI). If the WRAP inventory is not delivered in a timely manner, the Contractor will be able to use the NEI to proceed with this project until the necessary inventories are provided.

To use SMOKE for this subtask, the Contractor will modify scripts from previous work with the NEI and CMAQ, providing an efficient approach. These scripts use SMOKE to create CMAQ input files for each day of 1996, and run the latest SMOKE QA software to create reports at each stage of the processing. These SMOKE scripts will need to be configured differently for REMSAD than for CMAQ, so that they (1) create a separate elevated point-source file needed for REMSAD and not perform plume rise calculations in SMOKE, (2) output UAM-V format needed by REMSAD, (3) use REMSAD speciation profiles, and (4) use the latitude-longitude REMSAD grid definition and input files. These script changes require a minimal amount of effort.

In addition to changing our available scripts, the Contractor will create several ancillary SMOKE input files. The Contractor will start with the files created and tested for EPA, which work with the NEI. These files will be updated to include any state- or tribe-specific data. The Contractor will use existing software to remap the 36-km Lambert gridding surrogates to the 36-km latitude-longitude surrogates needed for the REMSAD version of the domain. The Contractor will do the same remapping of the biogenic land use using existing software as well. For chemical speciation and particulate splits, the Contractor will create REMSAD-specific speciation profiles based on those profiles used for CMAQ and from the appropriate data in EPA's SPECIATE model [http://www.epa.gov/ttn/chief/software/speciate/index.html].

The WRAP will supply all available inventory information for Canada and Mexico. In the event the WRAP inventory does not adequately cover Canadian sources, the Contractor will substitute the latest Canadian inventory available.

The Contractor will use current SMOKE scripting conventions to create the REMSAD emissions and QA reports. The Contractor will use comparisons of the reports with the raw inventory state and county totals to ensure that emissions are not dropped during the processing. The Contractor will use other types of totals (such as by source category code or by gridding surrogate code) to determine why any emissions results appear out of the ordinary. The Contractor will make qualitative analyses on the spatial and temporal allocation of the emissions through visualizations of the data, which will identify quantitative problems that we can investigate with SMOKE reporting tools.

The deliverables for this subtask are (1) all SMOKE input files used for this subtask; (2) all SMOKE outputs for use in REMSAD; (3) all QA reports; (4) all SMOKE software and supporting software (for format conversions, grid-to-grid transforms, etc.); (5) run scripts; and (6) documentation on methods used, quality assurance and inventory summaries, and use of any run scripts and QA software. These deliverables are intended to allow the WRAP RMC to replicate and/or modify the SMOKE base case emissions file preparation.

Subtask 1.4: Run REMSAD for 1996

Lead: ENVIRON

The purpose of this subtask is a successful base-year (1996) simulation for development and analysis of SIPs and TIPs. A good base-year simulation is needed to provide a credible starting point for future-year model simulations and analyses. To complete this subtask, the Contractor will (1) prepare additional REMSAD inputs other than the emissions and meteorology; (2) run the 1996 base case with the most current version of REMSAD provided by EPA; (3) update REMSAD postprocessing software necessary for the model performance evaluation, analyses, and QA; and (4) quality assure the base case simulation. A detailed model performance evaluation will be conducted in Subtask 1.5.

The additional inputs in item (1) include input data files specifying the initial species concentration fields (AIRQUALITY), lateral species concentrations (BOUNDARY), and gridded land use characteristics (SURFACE). Gridded fields of terrain elevations are not required because of the terrain-following sigma-P vertical coordinate system. The Contractor has previously created these files for EPA's ongoing continental U.S. modeling, but these

existing files may not be appropriate for the Western modeling domain. The Contractor will review and modify these files as needed, with particular emphasis on the boundary species concentration at the eastern edge of the domain

Deliverables for this subtask will include (1) all additional input data files for the 1996 annual REMSAD simulation, (2) the base case model output data files and the results of the QA/QC process in the form of statistical and graphical summaries, (3) new and/or enhanced software used for generation of input data and extraction of model outputs, and (4) sample job scripts used in each step of this subtask. These deliverables are intended to allow the WRAP RMC to replicate and/or modify the REMSAD base case simulations.

Subtask 1.5: REMSAD evaluation using the IMPROVE database

Lead: ENVIRON

The objective of this subtask is to perform a thorough model performance evaluation of the REMSAD 1996 model run, resulting in a credible base case simulation. For this subtask, the Contractor will (1) acquire and process the 1996 IMPROVE database; (2) acquire and process other available databases (listed in Section **Error! Reference source not found.**) as needed to provide sufficient model performance evaluation; (3) perform the multilevel model performance evaluation based on the approach outlined in the EPA and API PM modeling guidance; and (4) prepare an interim model performance evaluation report suitable for inclusion in the Task 1 final report.

The model performance evaluation will be conducted using a multilevel approach, as discussed above in Section **Error! Reference source not found.** . For this subtask the Contractor will focus on the operational and diagnostic evaluations previously described. The Contractor will also perform some mechanistic evaluation for emissions sensitivity and uncertainties.

The evaluation performed in step 3 above will be extended to the specific requirements of the regional haze initiative (i.e., it will focus on the 20% best- and worst-visibility days). The Contractor will evaluate the modeling system across the entire year because it provides a more robust evaluation and because a different set of days may make up the 20% best/worst days in the current and future years. The evaluation will pay special attention to data for the 16 GCVTC Class I areas. The comp lete evaluation approach will be described in detail in the modeling protocol and will include at least the following:

- Evaluation of the REMSAD-predicted concentration fields for reasonableness
- Evaluation of extinction across all days of the year and sites as well as for the 20% best and worst visibility days at each site
- Evaluation of extinction across all days and for the 20% best/worst days across all sites and for each site

Deliverables under this subtask will include (1) all software developed for processing the IMPROVE and other databases; (2) the extracted REMSAD modeling results required for the evaluation, and the results of the REMSAD model performance evaluation; and (3) an interim model performance evaluation report. All deliverables will be submitted to both the WRAP Modeling Forum and the RMC.

Subtask 1.6: Prepare future-year (2018 or 2020) model-ready base case emissions inventory

Lead: MCNC

The purpose of this subtask is to generate emission inputs for a future-year REMSAD model run for all of 1996. The WRAP inventory contractor will prepare the future-year inventory for input to SMOKE, so that SMOKE will not need to be used to project the emissions to the future year. To accomplish this subtask, the Contractor will (1) obtain and reformat (if necessary) the future-year WRAP inventory; (2) create run scripts from those created in Subtask 1.3 to run the future-year emissions; (3) run SMOKE for all days in 1996 (including generating QA reports); (4) quality assure SMOKE outputs, correct inputs, and rerun as necessary; and (5) document all processing steps and provide an interim report on the emission inputs for REMSAD, suitable for including in the Task 1 final report.

This subtask will be very straightforward because it will require only a minor modification to configure any SMOKE scripts to use a future-year inventory from what has been set up in Subtask 1.3. The deliverables for this subtask are analogous to those in Subtask 1.3, but all configured for the future-year run.

Subtask 1.7: Run REMSAD for future-year base case

Lead: ENVIRON

Under this subtask, the Contractor will set up and run REMSAD for the future-year base case using the model-ready emissions files developed under Subtask 1.6. The simulation will make use of the same meteorological and other input data developed in preceding subtasks. Model output data will be extracted for analyses and assessment of subsequent emissions control strategies. This subtask will make use of the software utilities and procedures developed for the 1996 baseline simulation and therefore can be performed efficiently and with a minimum of resources.

Deliverables will include (1) archived model output data files from the future-year simulation, (2) run scripts, and (3) documentation on how to reproduce the model runs. These will be submitted to both the Modeling Forum and the RMC.

Subtask 1.8: Compare future-year results against 1996 base case

Lead: ENVIRON

The objective of this task is to perform a comparison of the future-year base case with the 1996 baseline REMSAD model simulations. As described in the RFP, a similar comparison and assessment of the future-year GCVTC strategy simulation is also to be performed. Consequently, the Contractor will combine the activities called for in this subtask, as well as related costs, with the assessment specified in Subtask 1.11.

Subtask 1.9: Prepare future-year gridded model-ready inputs for GCVTC emissions

Lead: MCNC

The purpose of this subtask is to create the layer-1 and elevated REMSAD emission input files for the future-year control strategy. The GCVTC control strategy will be completely described to the Contractor. To accomplish this subtask, the Contractor will (1) create the SMOKE control input files based on the GCVTC control-strategy description; (2) create run scripts from those created in Subtask 1.3 to run the control-strategy emissions; (3) run SMOKE for all days in 1996 (including generating QA reports); (4) quality assure SMOKE outputs, correct inputs, and rerun as necessary; and (5) document all processing steps and provide an interim report on the emission inputs for REMSAD, suitable for including in the Task 1 final report.

As part of this task, the Contractor will ensure that the overall emission changes intended by the control strategy have been applied to the inventory. The most involved part of this subtask is preparation of the SMOKE control input files, because the script setup and script usage to run SMOKE will be very similar to previous subtasks. The deliverables for this subtask are analogous to those in Subtask 1.3, but all configured for the control-strategy run.

Subtask 1.10: Run REMSAD for GCVTC strategy

Lead: ENVIRON

Under this subtask, the Contractor will set up and run REMSAD for the future-year GCVTC strategy emission scenario using the model-ready emissions files developed under Subtask 1.7. The simulation will use the same meteorological and other input data developed in preceding subtasks. Model output data will be extracted for analyses and assessment of visibility impairment in support of the regional haze rule requirements. This task will make use of the software utilities and procedures developed for the 1996 baseline simulation and therefore can be performed efficiently and with a minimum of resources.

Deliverables will include (1) archived model output data files from the future-year GCVTC strategy simulations, (2) run scripts, and (3) documentation on how to reproduce the model runs. These will be submitted to both the Modeling Forum and the RMC.

Subtask 1.11: Assess visibility changes between 1996 base case and future-year emission scenarios

Lead: ENVIRON

For this subtask, the Contractor will assess the changes in visibility among the 1996 base case, the future-year base case, and the GCVTC strategy at each Western Class I area. The comparison of the 1996 base case and future-year base case will be performed as part of this task instead of Subtask 1.8, to be more cost efficient. The Contractor will give particular emphasis to the 16 GCVTC Class I areas with respect to visibility impairment. In particular, the Contractor will analyze the changes in light extinction of the mean of the 20% best and worst days at each of the Class I areas, and this analysis and related documentation will follow EPA's Fine Particulate Modeling Guidance. The Contractor will assess visibility measures using the light extinction algorithms and the monthly f(RH) values, as suggested by EPA. The Contractor will also perform additional analyses that will be detailed in the REMSAD modeling protocol. Finally, the Contractor will document the results of the assessment in an interim report suitable for inclusion in the Task 1 final report.

Deliverables under this task will be (1) results of the comparison of the 1996 and future-year base case REMSAD simulations, (2) results of the assessment of visibility impacts for the future-year base case and the GCVTC strategy simulations, and (3) an interim report that documents the approach, methodologies, and instructions for reproducing the analyses.

Subtask 1.12: Prepare final report

Lead: ENVIRON

The purpose of this task is to produce a final report documenting the Task 1 activities and analyses. The Contractor will prepare and submit a draft final report integrating the information contained in the subtask interim reports, including the base case model performance evaluation and the future-year base case and control-strategy assessments. Upon receipt of comments from the WRAP Modeling Forum on the draft, a Task 1 final report incorporating these comments and recommendations will be prepared and submitted for approval. The Task final report is the deliverable for this subtask, and it will also be included as part of the project's final report (Subtask 4.2).

All inputs, scripts, results, and documentation from Task 1 will be provided to the WRAP RMC as part of Task 3.

TASK 2: Set up, run, and assess Models-3/CMAQ for January and July 1996 using 1996 MM5 meteorological fields

Discussion: The subtasks described in this section all work toward providing credible Models-3/CMAQ simulations for January and July 1996. The analyses from Task 2 are relevant to development of the Section 308 SIPs and TIPs due in 2008.

For a project with near-term deadlines such as this one, it is very important to distinguish between Models-3 and CMAQ. Models-3 is a framework that provides a user interface for using many air quality components, including the CMAQ modeling system. On the other hand, the CMAQ modeling system is a collection of air quality modeling components that can be run from scripts or from the Models-3 interface.

MCNC has had some success with running the Models-3 framework, but so far it has not been acceptable for production runs like those needed in this project. With the recent release of an NT version of Models-3, the framework is supposedly more accessible and easier to set up. Given the intense time frames of this project and the available funds, however, we will plan on meeting the goals of this project by using CMAQ with scripts rather than with the Models-3 framework. Unsuccessful attempts to use the Models-3 framework will thus not hold back the project. The choice to use scripts should not be a problem, since the task is oriented more towards getting CMAQ set up and evaluated for the WRAP region than towards how those results will be obtained.

Subtask 2.1: Develop a CMAQ modeling protocol

Lead: MCNC

In this subtask the Contractor will develop a CMAQ modeling protocol and coordinate this work with Subtask 1.1 to ensure consistent modeling protocols for both REMSAD and CMAQ, to the extent possible. To best accomplish this subtask, the Contractor will first prepare a draft modeling protocol for review and comments by the WRAP Modeling Forum. Upon receipt of comments, the Contractor will revise the draft document to incorporate them and then submit the final CMAQ modeling protocol.

In preparing the modeling protocol, the Contractor will consider the issues described in Section **Error! Reference source not found.**. In summary, the CMAQ modeling protocol will be a map for ensuring the Contractor reaches the goal of providing detailed analyses relevant to the development of Section 308 SIPs and TIPs, due in 2008, and for providing comparisons to the REMSAD modeling in support of Section 309 SIPs and TIPs. WESTAR will facilitate modeling protocol development by communicating with the states and tribes and ensuring that the rest of the team is fully aware of the local issues of concern. The modeling protocol will describe in detail how the 1996 hourly 36-km CMAQ inputs will be developed, including meteorology, emissions, and ancillary inputs. It will also describe the procedures to be followed in conducting the CMAQ model performance evaluation.

The deliverables for this subtask will be a draft and final CMAQ modeling protocol submitted to the WRAP Modeling Forum and the RMC.

Subtask 2.2: Acquire and process MM5 meteorological fields for input to CMAQ for January and July 1996

Lead: MCNC

The purpose of this subtask is to provide the meteorology inputs for the January and July CMAQ episodes. The Contractor will (1) process the MM5 data through the Models-3 Meteorology-Chemistry Interface Processor (MCIP) for input to CMAQ, including domain subselection; (2) quality assure the meteorology inputs, and the results of the vertical layer collapsing in particular; and (3) document methods, quality assure results, and instructions on how to preprocess the MM5 data for the West to supplement the Models-3 guidance.

Since the Contractor already has the MM5 data readily available (project MC-14), this will provide an efficiency and cost savings for part (1) of this subtask. MCIP will be configured to extract the horizontal and vertical grids from the MM5 data files and to create the meteorological inputs to SMOKE and CMAQ (these share the same meteorology input format). MCIP has several different science algorithms options for processing the MM5 data, and the Contractor will determine the most appropriate choice for these settings and document this in the modeling protocol.

The deliverables for this subtask are (1) the CMAQ meteorology input files; (2) the MCIP run scripts; (3) the results of the QA measures and other supporting results such as log files; and (4) an interim report that documents the approach and instructions for reproducing the preprocessing and analysis, suitable for including in the Task 2 final report.

Subtask 2.3: Process best-available WRAP emissions inventory through SMOKE for input to CMAQ for January and July

Lead: MCNC

The purpose of this subtask is to create emission inputs for use with CMAQ for the two one-month simulations. To accomplish this subtask, the Contractor will (1) create speciation input files, gridding surrogates, and gridded land use data appropriate for the CMAQ simulation; (2) create run scripts from our existing CMAQ annual run scripts, suitable for the Western domain; (3) run SMOKE processors needed for CMAQ-specific runs where steps are different from the Task 1 REMSAD basecase run (including generating QA reports); (4) quality assure SMOKE outputs, correct inputs, and rerun as necessary; and (5) document all processing steps, processing and data decisions, and provide an interim report on the emission inputs for CMAQ, suitable for including in the project final report for Subtask 4.2.

Because of SMOKE's modular structure, many of the emissions processing steps needed for this subtask will have already been completed in Task 1. The 1996 base case inventory used in Task 1 will also be used here. For each source category, the Contractor will therefore need to rerun the SMOKE speciation module for the different CMAQ speciation, the gridding module for the CMAQ grid, the layer fractions program (because CMAQ requires plume rise to be computed before input), the merge module for creating the model-ready files, and the reports module for generating CMAQ-specific reports for quality assurance and summary purposes. The exception to this run structure is biogenic processing: all biogenic steps will need to be rerun for this subtask. This strategy will ensure that the same inventory is used for both the REMSAD and CMAQ runs, which will be necessary for comparing results from the two models.

The QA techniques that the Contractor will use in this subtask were summarized previously in Subtask 1.3.

The deliverables for this subtask are (1) all SMOKE input files used for this subtask; (2) all SMOKE outputs for use in CMAQ; (3) all QA reports; (4) all SMOKE software and supporting software (for format conversions, grid-to-grid transforms, etc.); (5) run scripts; and (6) documentation on methods used, quality assurance and inventory summaries, and use of any run scripts and QA software. These deliverables are intended to allow the WRAP Modeling Forum and the WRAP RMC to replicate and/or modify the SMOKE base case emissions file preparation.

Subtask 2.4: Run CMAQ for January and July

Lead: MCNC

The purpose of this subtask is to create credible January and July model runs for the 1996 base case using CMAQ. The Contractor will use the meteorology and emissions input files created in Subtasks 2.2 and 2.3. To complete this subtask, the Contractor will (1) benchmark CMAQ on the computing platform selected and specified in the modeling protocol, (2) create the initial and boundary conditions files and create the clear sky photolysis rate table, (3) create and set up the software needed for the model performance evaluation and quality assurance, (4) test model optimization and configuration options to determine the final configuration to be documented in the modeling protocol, and (5) quality assure the CMAQ model runs.

Through the draft modeling protocol, the Contractor will present the WRAP Modeling Forum with multiple options for the IC/BC files for initializing the simulations. The Contractor will use the most current set of photolysis rate data that match the CMAQ photochemical mechanism used in this project to create the clear-sky photolysis rate look-up table used by CMAQ. The Contractor will finalize the IC/BC files and photolysis inputs before the final model runs for January and July, and the methods and reasons for using these data will be documented in the interim report for this subtask.

In the modeling protocol, the Contractor will also present several CMAQ model configuration and scripting options that the Contractor will investigate to determine a final model configuration. The Contractor will document any differences in CMAQ results and performance due to the level of optimization used in compiling CMAQ.

The deliverables for this subtask will be (1) all additional input data files for the January and July 1996 CMAQ simulations, (2) the base case model output data files and the results of the QA/QC process in the form of statistical and graphical summaries, (3) new and/or enhanced software used for generation of input data and extraction of model outputs and quality assurance, and (4) sample job scripts, and log files created in each step of this subtask. These deliverables are intended to allow the WRAP Modeling Forum and the WRAP RMC to replicate and/or modify the CMAQ January and July simulations.

Subtask 2.5: Assess CMAQ results through comparison to IMPROVE data and to REMSAD results

Lead: MCNC

The purpose of this subtask, through iterations with Subtasks 2.4 through 2.7, is to evaluate CMAQ model performance for January and July of 1996 and achieve reasonable model performance. Unlike REMSAD, which has a good history of use in the community, CMAQ is a larger unknown. Consequently, the Contractor propose to begin model testing using two10-day test periods, in January and July, which will allow many issues to be resolved without the more time-consuming task of running and analyzing CMAQ for two entire months. These "shake-down"

runs will help identify any gross errors in the input data or the model itself, will provide a preliminary assessment of the performance of the model, and will enable revisions and development of a rigorous modeling protocol.

The shake-down runs will not replace the full model evaluation; rather, they will provide a more efficient mechanism for completing the two-month model evaluation. Under no circumstances will we fail to create the January and July simulations. This approach will span a number of tasks. The following is an outline of the steps that to be taken for Subtasks 2.4 through 2.7. These steps will occur together in an iterative fashion with the ultimate objective of January and July model performance evaluations of CMAQ.

10-day shake-down simulations

- Run CMAQ for 10-day periods in January and July (Subtask 2.4)
- Evaluate results using internal consistency checks, limited comparisons to ambient measurements, and comparison with the REMSAD results as described in Section **Error! Reference source not found.** (Subtask 2.5)
- Assess model performance based on above evaluations and make recommendations to the WRAP Modeling Forum about changes to the model inputs and model configuration (Subtask 2.6)
- Update model configuration, emissions, and/or other model inputs based on previous evaluations (Subtask 2.7)
- Repeat as needed until comfortable with trying the month-long simulations (Subtask 2.7)

Full month-long simulations

- Run CMAQ for full-month January and July simulations (Subtask 2.4)
- Perform internal consistency check, comparisons to ambient measurements, and comparisons with REMSAD results as described in Section **Error! Reference source not found.** (Subtask 2.6)
- In addition, perform all evaluations and analyses to create complete model performance evaluation (Subtask 2.8).

The model evaluations will use techniques described in Section **Error! Reference source not found.** . These evaluations will include the operational, diagnostic, and mechanistic evaluations described in that section. The full-month runs will obviously provide larger model data sets for analysis of trends than the shake-down runs. The Contractor will apply the many types of approaches previously summarized for internal consistency checks, comparisons with IMPROVE and other observational data, and intermodel comparisons.

The deliverables iteratively obtained from this subtask will be the (1) final results of CMAQ assessment from comparison to IMPROVE and other observational data and comparison to the REMSAD results, (2) final datasets and software used to perform model assessment, and (3) final documentation on how to perform analyses. These deliverables are intended to allow the WRAP Modeling Forum and the WRAP RMC to replicate and/or modify the CMAQ January and July simulations.

Subtask 2.6: Assess system performance and recommend changes to the modeling input data and/or the modeling system

Lead: MCNC

The purpose of this subtask is to use the model performance evaluations from Subtask 2.5 to determine changes to the modeling input data and/or the air quality model. This subtask will be performed based on the shake-down simulations. Common errors in input data include poor spatial or temporal allocation of emissions for one or more model species, inappropriate boundary or initial conditions, and meteorology that is inconsistent with observations.

Deliverables for this subtask are several interim reports that summarize our findings about system performance and make recommendations on how to improve the modeling system. The Contractor will coordinate with the WRAP Modeling Forum to get feedback on these recommendations before implementing any proposed changes.

Subtask 2.7: Make changes and rerun as necessary

Lead: MCNC

The purpose of this subtask is to improve the modeling system to achieve acceptable model performance. In this project, the Contractor will be able to modify emissions data, initial and boundary conditions, the MCIP processing, SMOKE, CMAQ, and the postprocessing and analysis methods. While the Contractor will be able to identify and recommend changes to the meteorology, rerunning MM5 is outside the scope of this project, so will need to work within the MM5 data limitations that exist. This subtask will require (1) coordination between the emissions processing, meteorology preprocessing, CMAQ model runs, and postprocessing, (2) updating the necessary system components, and (3) documenting updates and iterations. The model runs take place under Subtask 2.4.

The changes and recommendations for this subtask will be based on the shake-down simulations. The full evaluation of the model from the two full-month simulations will be limited to a single run, barring glaring input errors (e.g., missing or wrong input files). If the Contractor encounters an exceptionally poor initial model performance from CMAQ, the Contractor will identify the weaknesses in the system, including the following:

- Unrepresentative meteorology
- Poor emissions estimates or poor spatial or temporal distribution of emissions
- Errors in model coding or configuration

Since the final inputs and CMAQ runs will be delivered under Subtask 2.5, the deliverables for this subtask is documentation on the changes made and methods used to make the changes.

Subtask 2.8: Complete model performance evaluation for January and July CMAQ results

Lead: MCNC

This subtask is an endpoint to the iterative process of model performance evaluation and improvement. For this subtask, the Contractor will perform all of the analyses used to assess the shake-down runs and also add the more complete analyses and summaries suitable for a project final report (Subtask 4.2). The deliverable from this subtask is an interim report, which will include descriptions of the final model configuration, the modeling issues that were resolved, the outstanding issues that were not resolved, recommendations for further improvements to the system, and the model performance analyses and results. The Contractor will submit the interim report to the WRAP Modeling Forum for review, and we will include comments on it in the project final report.

TASK 3: Provide technical guidance to the WRAP Regional Modeling Center and transfer all relevant files, programs, and documentation to the WRAP

Subtask 3.1: Develop data archiving and transfer plan

Lead: MCNC

Both MCNC and ENVIRON have substantial capabilities for data archiving, creating tapes and other data transfer mechanisms, and creating web pages to communicate with clients. The Data Migration Facility (DMF) at MCNC currently manages about 42 terabytes of data. It uses a robot to automatically store on tape two versions of all data files submitted to the system. This facility is a substantially more efficient and durable way of archiving large amounts of data than using tapes alone. MCNC typically automates the archiving of model results to DMF and in many cases the creating of web pages for online, password-protected display of data for clients. DMF will permit us to provide access to the results of the project for up to three years, as needed.

In this subtask, the Contractor will utilize these resources to develop a custom data archiving and transfer plan that meets the needs of the WRAP Modeling Forum, Emissions Forum, and RMC. Some of the issues that the Contractor will consider are the amount of data to be archived, the regularity with which data are stored, convenience of access to these data by outside stakeholders, efficiency and quality of transfer of the data to the RMC. The Contractor will archive all model inputs, outputs, and system configuration information from both ENVIRON and MCNC. Towards

the start of the project, the Contractor will create a draft data archiving and transfer plan. The Contractor will supply this draft to the WRAP, address comments, and include the resulting information in both the final modeling protocols and the project final report.

Subtask 3.2: Provide technical support to the Regional Modeling Center for setup of REMSAD and Models-3/CMAQ

Lead: MCNC

A primary objective of this project is providing a jumpstart on the modeling efforts for the RMC. This subtask specifically addresses the need for this project to support the RMC with setup and use of the REMSAD and Models-3/CMAQ systems. The Contractor will to provide technical support for REMSAD and Models-3/CMAQ in the following ways:

1. Install and test installation packages created in Subtask 3.3 at RMC facilities through remote installation.
2. MCNC will offer in-kind support for SMOKE, REMSAD, and Models-3/CMAQ for a period of one month at some point after the end of this project (to be determined by the RMC). The Contractor will determine what components of the RMC will have access to this support once the RMC has been identified. This support will include:
    - Providing and installing updates of the software available through other mechanisms
    - Technical support via phone, e-mail, and documentation on the web site

Subtask 3.3: Provide technical transfer support of all modeling and analysis tools to the Regional Modeling Center

Lead: MCNC

The purpose of this subtask is to provide all results from this project to the WRAP RMC. To accomplish this subtask the Contractor will (1) implement the data archiving and transfer plan from Subtask 3.1; (2) create distribution tapes containing all model inputs, outputs, log files and automatic reports, all modeling software, pre- and postprocessors, scripts, and documentation necessary to perform the analyses from Tasks 1 and 2; (3) deliver the distribution tapes to the WRAP Modeling Forum and deliver and install these for the RMC; (4) provide a one-day technical workshop for the RMC members and any WRAP participants to attend, to be held after the final project presentation to the WRAP RMC; and (5) work with the RMC to assure that they are able to operate SMOKE, REMSAD, MCIP, and CMAQ.

The distribution tapes will provide the various modeling systems as a turnkey system with scripts designed to operate using a Unix or LINUX computing environment. For REMSAD, the Contractor will also provide example problems and scripts for generating all of the REMSAD inputs. These include the MM5/REMSAD processor that was used previously to create the REMSAD 36-km 8-layer modeling inputs.

The technical workshop will provide a more detailed perspective of all of the models and analyses that were used to accomplish this project. It will significantly assist the RMC in picking up where this project leaves off. The Contractor will help the RMC to understand the science and technology behind SMOKE, REMSAD, MCIP, and CMAQ (e.g., assumptions that are used in the REMSAD visibility postprocessor). The Contractor will have this workshop at the same facility that the WRAP selects for the final presentation.

The deliverables from this subtask are (1) the distribution tapes and the installation of these tapes for the RMC, and (2) a one-day workshop for the RMC and WRAP participants.

TASK 4: Reporting and communication

Discussion: Providing reports, analysis, and other documentation to clients on a web site is an extremely efficient and effective mechanism for distribution of information. MCNC has been successfully using a web site to communicate modeling results to the North Carolina Department of Environment and Natural resources (project MC-3). In addition to the specific mechanisms in the RFP, the Contractor will overlay these mechanisms on a web

site that we will create for this project. This web site can be password protected if necessary. The Contractor will work with the WRAP Modeling Forum and RMC to develop optimal methods of communication.

The Technical Workshop described in Subtask 3.3 is an additional form of communication that has been added to supplement to those listed in the RFP.

Subtask 4.1: Communicate results to the WRAP Regional Modeling Center and the Modeling Forum

Lead: MCNC

Excellent communication is an essential aspect of a successful project. All deliverables will be geared towards communication with the Modeling Forum and/or the RMC.

Subtask 4.1.1: Biweekly conference calls

MCNC will initiate and participate in biweekly conference calls. These calls will provide a forum for brief updates on the status of the project, a mechanism to address issues or concerns of the WRAP Modeling Forum, and a way for the project team to receive feedback on interim reports. Materials needed for discussion on the conference calls will be posted on the web site.

1.1.1.1 Subtask 4.1.2: Written monthly status reports or memoranda

As described in the tasks above, the Contractor will create many interim reports to provide a useful way to formally collaborate with the WRAP Modeling Forum. In addition to these, briefer monthly reports summarizing the project status will be provided to the Modeling Forum. These reports will summarize the issues from the biweekly conference calls, and provide building blocks for the final report. These reports will be available on the project web site.

1.1.1.2 Subtask 4.1.3: Two presentations to the WRAP Modeling Forum

The Contractor will attend the WRAP Modeling Forum meetings to provide presentations on the project. The first presentation will be at the midpoint of the project, and the second at the end of the project. Both MCNC and ENVIRON will attend these presentations. ENVIRON has attended two WRAP Modeling Forum meetings in the past using internal funding. ENVIRON would continue to use internal funding to attend one of the two meetings under this task as part of their in-kind support to the WRAP modeling efforts. In these presentations, the Contractor will present the results of the project and receive feedback from the WRAP Modeling Forum. The presentation materials and summaries of discussions will be posted on the project web site.

Subtask 4.2: Generate a final report describing all relevant aspects of the analysis

Lead: MCNC

MCNC and ENVIRON will combine all of the interim reports and monthly reports to create a coherent final report for the project. This report will include all of the relevant analyses used in generating the three REMSAD simulations and the CMAQ model performance evaluation.

The user instructions for replicating the analyses and using the systems provided with the distribution tapes will be provided in a separate document compiled as part of Subtask 3.3.