User's Guide to the Regional Modeling System for Aerosols and Deposition (REMSAD)

Version 7

July 2002

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1. INTRODUCTION

This document is intended to serve as guide to the application of the Regional Modeling System for Aerosols and Deposition (REMSAD), and specifically version 7 of the modeling system. First time users of the REMSAD modeling system should read the entire document prior to commencing their work, as it provides important and useful information related to the set up of a new application, computer resource requirements, and input parameter specifications. Experienced users of the REMSAD modeling system may wish to reference only specific sections of the document. To accommodate this, those sections describing the technical formulation, input and output files, and postprocessing procedures are written (to the extent possible) such that they can be used independently (in the spirit of a quick reference guide). Thus, some of the information contained in this document (when read in its entirety) may seem repetitive.

The REMSAD modeling system was developed and is maintained and distributed by Systems Applications International, Inc. (SAI), a wholly owned subsidiary of ICF Consulting. The U.S. Environmental Protection Agency (EPA) funded major portions of the development of REMSAD.

The REMSAD modeling system was originally intended as a screening tool—a model that could be run (quickly) for a continental-scale modeling domain (specifically the continental U.S) and for a full-year simulation period—to provide information (although not very detailed) on the distribution and composition of particulate matter, the deposition of pollutant (including toxic) species onto the surfaces of inland and coastal bodies of water, and the expected change in air quality and deposition that results from changes in emissions. All of these parameters were intended to be primarily represented in terms of seasonal or annual averages or deposition totals. What began as a simple screening tool has evolved into a more complex modeling system that attempts to simulate the chemistry, transport, and deposition of airborne pollutants (with emphasis on particulate matter (PM), ozone, and mercury) using algorithms that reflect the state-of-the science and current knowledge of the important physical and chemical processes.

The remainder of this section provides a brief overview of the modeling system and a discussion of the attributes and limitations of Version 7 of the REMSAD model. The technical formulation is described in more detail in Section 2 of the user's guide. General application procedures are summarized in Section 3. Input requirements and preparation procedures are described in Section 4. The content and format of the REMSAD output files is listed in Section 5. Finally, a discussion of standard postprocessing procedures is provided in Section 6.

1.1. Overview of the REMSAD Modeling System

The Regional Modeling System for Aerosols and Deposition (REMSAD) is designed to support a better understanding of the distributions, sources, and removal processes relevant to fine particles and other airborne pollutants, including soluble acidic components and toxics. Consideration of the different processes that affect primary and secondary (i.e., formed by atmospheric processes) particulate matter at the regional scale in different places is fundamental to advancing this understanding and to assessing the effects of proposed pollution control measures. These same control measures will, in most cases, affect ozone, particulate matter and deposition of pollutants to the surface.

The REMSAD system is built on the foundation of the variable-grid Urban Airshed Model (UAM-V)—a regional-scale photochemical modeling system (SAI, 1999). Thus many of features

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of the UAM-V are also available in REMSAD. The REMSAD model is capable of "nesting" one or more finer-scale subgrids within a coarser overall grid, which permits high resolution over source and/or receptor regions. The modeling system may be applied at scales ranging from a single metropolitan area to a continent containing multiple urban areas. To date, most applications have focused on the continental-scale. In addition, the model is typically exercised for a full year.

REMSAD is a three-dimensional grid model designed to calculate the concentrations of both inert and chemically reactive pollutants by simulating the physical and chemical processes in the atmosphere that affect pollutant concentrations. The basis for the model is the atmospheric diffusion or species continuity equation. This equation represents a mass balance in which all of the relevant emissions, transport, diffusion, chemical reactions, and removal processes are expressed in mathematical terms. The REMSAD system consists of a series of preprocessor programs, the core model, and several postprocessing programs.

Fine particles (or aerosols) are currently thought to pose one of the greatest problems for human health impacts from air pollution. The major factors that affect the concentration and distribution of aerosols include:

- Spatial and temporal distribution of toxic and particulate emissions including sulfur dioxide (SO_2), oxides of nitrogen (NO_x), volatile organic compounds (VOC), and ammonia (NH_3) (both anthropogenic and nonanthropogenic),

- Size composition of the emitted PM,

- Spatial and temporal variations in the wind fields,

- Dynamics of the boundary layer, including stability and the level of mixing,

- Chemical reactions involving PM, SO_2, NO_x and other important precursor species,

- Diurnal variations of solar insulation and temperature,

- Loss of primary and secondary aerosols and toxics by dry and wet deposition, and

- Ambient air quality immediately upwind and above the region of study.

The REMSAD model simulates these processes when it is used to simulate aerosol distribution and deposition. The model solves the species continuity equation using the method of fractional steps, in which the individual terms in the equation are solved separately in the following order: emissions are injected; horizontal advection/diffusion is solved; vertical advection/diffusion and deposition is solved; and chemical transformations are performed for reactive pollutants. The model performs this four-step solution procedure during one half of each advective (driving) time step, and then reverses the order for the following half time step. The maximum advective time step for stability is a function of the grid size and the maximum wind velocity or horizontal diffusion coefficient. Vertical diffusion is solved on fractions of the advective time step to keep their individual numerical schemes stable. A typical advective time step for coarse (50–80 km) grid spacing is 10–15 minutes, whereas time steps for fine grid spacing (10–30 km) are on the order of a few minutes.

Model inputs are prepared for meteorological and emissions data for the simulation days. Once the model results have been evaluated and determined to perform within prescribed levels, a *projected* emission inventory can be used to simulate possible policy-driven emission scenarios.

REMSAD provides gridded, averaged surface and multi-layer instantaneous concentrations, and surface deposition output for all species and grids simulated. The averaged surface concentrations and depositions are intended for comparison with measurements and ambient standards. The instantaneous concentration output is primarily used to restart the model, and to examine model results in the upper levels. Concentrations of particulates are passed as input to a postprocessor module that estimates atmospheric visibility. Wet and dry deposition fluxes are calculated hourly and may be accumulated for any desired interval.

The particulate matter species modeled by REMSAD include a primary coarse fraction (corresponding to particulates in the 2.5 to 10 micron size range), a primary fine fraction (corresponding to particulates less than 2.5 microns in diameter), and several secondary particulates (e.g., sulfates, nitrates, and organics). The sum of the primary fine fraction and all of the secondary species is assumed to be representative of $PM_{2.5}$. This is calculated as part of a postprocessing step.

The photochemical mechanism module used in REMSAD is a reduced-form version of Version 4 of the Carbon-Bond Chemical Mechanism (CB-IV) (Gery et al., 1989) as enhanced to include radical-radical termination reactions. This reduced-form version is termed "micro-CB-IV" and is based on a reduction in number of different organic compound species that are included. The inorganic and radical parts of the mechanism are identical to CB-IV. The organic portion of the chemistry is based on three primary organic compound species (VOC representing an average anthropogenic hydrocarbon species, and ISOP and TERP—representing biogenic hydrocarbon species) and one carbonyl species (CARB).

Secondary organic aerosol species (SOA) are known to result from the reactions of hydrocarbons in the atmosphere. REMSAD Version 7 includes a calculation of the yield of SOA from both anthropogenic and biogenic hydrocarbon species. Of the anthropogenic hydrocarbon emissions, the aromatic hydrocarbons are the principal contributors to SOA. Therefore, a provision is included in REMSAD to establish the aromatic fraction of VOC as a function of space and time. Biogenic emissions the species TERP, representing monoterpenes, which are the principal biogenic precursors of SOA.

REMSAD simulates both wet and dry deposition of gaseous and particulate species. Wet deposition occurs as a result of precipitation scavenging. Dry deposition is calculated for each species based on land-use characteristics and meteorological parameters.

The chemical transformations of mercury included in Version 7 of REMSAD are based on the review of current status of atmospheric chemistry of mercury presented by Lin and Pehkonen (1999). Prior versions of REMSAD included only the aqueous phase reaction of mercury with ozone. Species representing the oxidation state of mercury and the phase (gas or particulate) are tracked. These include HG0 (elemental mercury vapor), HG2 (divalent mercury compounds in gas phase), and HGP (divalent mercury compounds in particulate phase). A tagging scheme for the mercury (and other) species is an optional feature of REMSAD.

A number of issues are particularly important to a successful application of REMSAD for evaluating the atmospheric transport and deposition of pollutants. These include the accuracy and representativeness of the meteorological and emission inventory inputs; the resolution, structure and extent of the modeling grid; and the treatment of urban areas in both the source and receptor areas of the computational grid.

1.2. Use of REMSAD: Attributes and Limitations

The REMSAD modeling system provides a relatively simple and cost effective means to begin to study and understand, through modeling, the factors that contribute to PM, mercury, and toxics concentrations and deposition totals, and the relative effectiveness of emission reductions measures in reducing the associated air quality related values. Attributes of the REMSAD modeling system, relevant to its use for current air quality modeling studies, include the following:

- Since the REMSAD modeling system is based on the UAM-V modeling system framework, many existing datasets that were developed for ozone modeling can be readily adapted for use with REMSAD.

- Simplification of the photochemical and other processes enables one to use REMSAD to obtain regional and annual estimates of PM, visibility, and deposition using readily available (standard) computer technology in a reasonable amount of time (a typical continental-scale (for the U.S.), annual simulation takes about two weeks of computer run time on a high-end (by today's standards) work station).

- Despite the simplifications, many of the key features and components of the REMSAD model are consistent with the state-of-the-science knowledge and techniques as related to particulates, mercury, and other toxic species (as discussed in more detail in Section 2 of the user's guide).

- Results from numerous applications of REMSAD (conducted by SAI and EPA) as well as a peer-review of the modeling system (Seigneur et al., 1999) have demonstrated that the modeling system can produce credible results and have led to testing and refinement of several of the modeling system components (that comprise version 7).

- Future versions of REMSAD will benefit from the insights and experiences of various members of the air quality modeling community, through their participation in a newly formed REMSAD user's group (see http://remsad.saintl.com for more information)

At this time, there is a lot that is still unknown about the formation, composition, transport, and deposition of particulate and toxic species. Version 7 of the REMSAD modeling system has several key limitations that should be considered prior to its use. These include:

- Simplified ozone chemistry may not adequately represent ozone concentrations as well as the interactions of ozone with other pollutant species (e.g., PM).

- REMSAD (Version 7) does not include a plume-in-grid treatment for the detailed treatment of plume chemistry and dynamics for large point sources.

2. TECHNICAL FORMULATION

The technical background for REMSAD is discussed in this section of the user's guide. Many of the features and algorithms are based on research as reported in published literature; in these cases the additional references are provided.

REMSAD is a three-dimensional, grid-based (or Eulerian) model designed to calculate the concentrations of both inert and chemically reactive pollutants by simulating the physical and chemical processes in the atmosphere that affect pollutant concentrations. The framework of the model (including the advection and deposition algorithms) is similar to that for the UAM-V regional-scale photochemical modeling system.

The basis for the REMSAD model is the atmospheric diffusion equation (also called the species continuity or advection/diffusion equation). This equation represents a mass balance in which all of the relevant emissions, transport, diffusion, chemical reactions, and removal processes are expressed in mathematical terms as follows:

$$\underbrace{\frac{\partial c_i}{\partial t}}_{\substack{\text{Time} \\ \text{Dependence}}} + \underbrace{\frac{\partial(uc_i)}{\partial x} + \frac{\partial(vc_i)}{\partial y} + \frac{\partial(wc_i)}{\partial z}}_{\text{Advection}} = \underbrace{\frac{\partial}{\partial x}\left(K_X\frac{\partial c_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_Y\frac{\partial c_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_V\frac{\partial c_i}{\partial z}\right)}_{\text{Turbulent Diffusion}}$$

$$+ \underbrace{R_i}_{\substack{\text{Chemical} \\ \text{Reaction}}} + \underbrace{S_i}_{\text{Emissions}} + \underbrace{D_i}_{\substack{\text{Dry} \\ \text{Deposition}}} + \underbrace{W_i}_{\substack{\text{Wet} \\ \text{Deposition}}}$$

where

c_i	=	concentration of pollutant i, a function of space (x,y,z) and time (t)
u,v,w	=	horizontal and vertical wind components
K_X, K_Y	=	horizontal turbulent diffusion coefficients
K_V	=	vertical turbulent exchange coefficients
R_i	=	net rate of production of pollutant i by chemical reactions
S_i	=	emission rate of pollutant i
D_i	=	net rate of change of pollutant i due to surface uptake processes
W_i	=	net rate of change of pollutant i due to wet deposition processes

Each of the terms in this equation represent different processes and are calculated for each time step using finite-difference numerical techniques, in which the derivatives in the equation are replaced by differences taken for discrete sets of points in space and time (i.e., grid cells and time steps). The REMSAD modeling domain and grid structure are specified by the user. The time step used in numerically solving the advection/diffusion equation is determined by the model, based on horizontal grid resolution and wind speed.

The processes as well as the key features of the REMSAD modeling system are described in the following sections, following an overview of the modeling system components and grid structures.

2.1. Modeling System Components and Key Features

A schematic diagram of the REMSAD modeling system is shown in Figure 2-1. The modeling system includes an atmospheric transport and deposition module (also referred to in the software as the ATDM), which is the core of the modeling system.

The REMSAD modeling system comprises a variety of emissions, meteorological, land-use, and chemistry input files. In total 17 files are required as input. Depending on the particular simulation options chosen and the species to be simulated, additional input files may also be required. Many of the input files are specific to the modeling domain and simulation period. The input files and preparation procedures are described in more detail in Section 4 of this user's guide.

Key features and capabilities of the modeling system include:

- Flexible horizontal and vertical coordinate system (with nested-grid capabilities and user-defined vertical layers).

- Reduced Carbon-Bond IV (CB-IV) gas phase chemistry (micro-CB-IV).

- Parameterized aerosol chemistry and dynamics for fine and coarse particles.

- Calculation of SOA yields from emitted hydrocarbons

- Simulated treatment of five toxic species (including cadmium, mercury, dioxin, polycyclic organic matter, and atrazine).

- Tagging scheme for cadmium and mercury.

Figure 2-1
REMSAD System
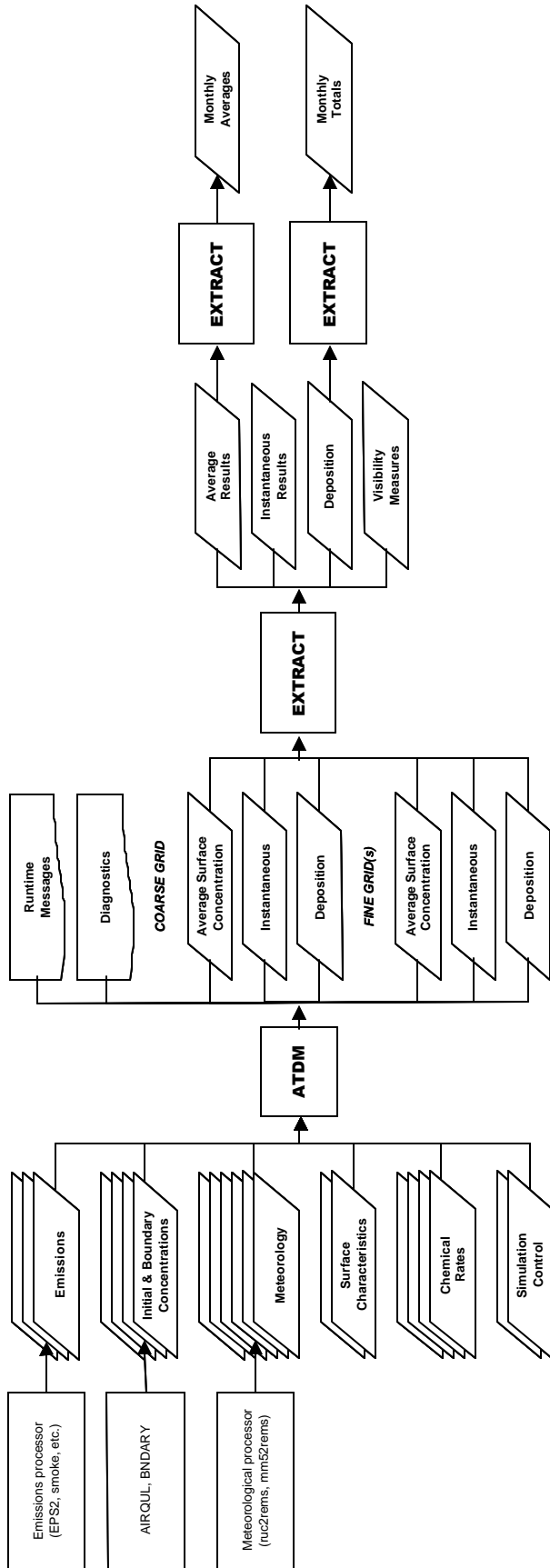
2.2. Horizontal and Vertical Coordinate Systems and Grid Structures

REMSAD is a grid-based modeling system in which a three-dimensional grid (comprised of both horizontal and vertical grid cells) is placed over the region of interest. Within this grid, finer, nested grids may also be defined for regions for which more refined analyses are desired. The REMSAD model supports nesting in both the horizontal and vertical dimensions.

2.2.1. Horizontal Coordinate System

The REMSAD model currently supports the use of a geodetic (latitude/longitude) horizontal coordinate system or a Cartesian horizontal coordinate system measured in kilometers. Using the geodetic coordinate system, the extent and structure of the horizontal grid is specified based on the latitude and longitude of the grid origin, the number of grid cells in the west-east and north-south directions, and the size of the grid cells in the west-east and north-south directions in units of degrees longitude and latitude, respectively.

When using a Cartesian coordinate system, the extent and structure of the horizontal grid is based on a grid origin (relative to some standard reference point), the number of grid cells in the west-east and north-south directions, and the size of the grid cells in units of km. The REMSAD system currently supports Cartesian grids based on the UTM system or Lambert conformal map projections.

2.2.2. Vertical Grid Structure

The vertical layer structure of REMSAD is defined in terms of sigma-pressure coordinates: $\sigma_p = (p - p_t)/(p_s - p_t)$, where p is pressure, p_t is the constant pressure specified as the top of the modeling domain, and p_s is surface pressure. The sigma levels follow the variable terrain and are specified by the user. It is recommended that the sigma layers be chosen to accommodate the mapping of the output from the meteorological model used for the application to the REMSAD vertical grid structure.

2.2.3. Grid Nesting

Grid nesting is a technique that is used to achieve a balance between grid extent and resolution. The extent of the model grid should be sufficient to accommodate the regional- or, in some cases, continental-scale transport of pollutants (perhaps especially important for simulating PM, regional haze, and mercury), while the resolution should support the accurate simulation of the important meteorological, chemical, and deposition processes. These two aspects of the modeling domain should be specified with regard to computational requirements. Since the amount of computer time required for a simulation is proportional to the number of grid cells, higher resolution typically means more computing time – unless the extent of the modeling domain is reduced accordingly. Grid nesting allows one to accommodate both regional and subregional influences as well as to provide a detailed representation of the emissions, meteorological fields, and pollutant concentration and deposition patterns over the primary area(s) of interest without the full computational burden that would accompany high resolution for the entire domain.

REMSAD employs a two-way nested-grid approach. The results for each outer grid influence each inner grid as boundary conditions, while the results for each inner grid are supplied to each outer grid for use in subsequent calculations. Nesting may be applied in both the horizontal and the vertical. In both cases, the fine grids must be nested completely within the coarse grid domain and the edges of the fine grid must correspond to a coarse grid cell edge. The horizontal spacing of a fine grid may be any integral subdivision of the coarser grid within which it is embedded. There may be multiple fine grids within a coarse grid, and there can be several levels of nesting (i.e., finer grids embedded within another fine grid); however, fine grids cannot overlap each other. The REMSAD nested-grid approach is identical to that used by the UAM-V which has been tested to assure accuracy and mass consistency.

Gridded low-level emissions input files must be supplied separately for the coarse and fine grids. Land-use, surface pressure, gridded ozone, wind, and vertical exchange coefficient input files may (optionally) be specified separately for the fine grids. If these are not provided, the information for the fine grids will be obtained by interpolation from the coarse-grid inputs. Other inputs, such as temperature and water vapor concentrations, are always interpolated by the model to the fine grids from the coarse grid inputs.

The species continuity equation using nested grids in REMSAD is solved as follows:

1. Emissions for a full time step are injected into the coarse grid.

2. Vertical diffusion, including dry deposition, is calculated for the coarse grid for one-half time step (note the time step for the coarse grid will be different from (and larger than) that for the fine grid).

3. Vertical advection is calculated for the coarse grid for one-half time step.

4. Horizontal advection and diffusion are calculated for the coarse grid for one-half time step.

5. For each fine grid:

   (a) The time step is set equal to an integral fraction of the coarse-grid time step (in accordance with grid cell size).

   (b) Emissions for one fine grid step are injected into the fine grid.

   (c) Vertical diffusion, including dry deposition, is calculated for the fine grid for one-half of a fine grid step.

   (d) Vertical advection is calculated for the fine grid for one-half of a fine grid step.

   (e) Horizontal advection and diffusion are calculated for the fine grid for one-half of a fine grid step.

   (f) Chemistry calculations (gas phase chemistry, aqueous phase chemistry, and toxics chemistry) and convective mixing calculations are carried out for the fine grid for a fine grid step.

   (g) Horizontal advection and diffusion are calculated for the fine grid for one-half of a fine grid step.

   (h) Vertical advection is calculated for the fine grid for one-half of a fine grid step.

(i) Vertical diffusion, including dry deposition, is calculated for the fine grid for one-half of a fine grid step.

(j) Steps (a) through (i) are repeated for a time period equal to a coarse-grid time step.

6. Chemistry calculations (gas phase chemistry, aqueous phase chemistry, and toxics chemistry) and convective mixing calculations are carried out, for those coarse-grid cells not covered by a fine grid, for a full coarse grid step. Convective mixing calculations include calculation of wet deposition.

7. Horizontal advection and diffusion are calculated for the coarse grid for one-half time step.

8. Vertical advection is calculated for the coarse grid for one-half time step.

9. Vertical diffusion, including dry deposition, is calculated for the coarse grid for one-half time step.

10. Coarse grid concentrations are updated with fine grid results.

When running simulations without fine grids, step 5 and all its sub-steps and step 10 are omitted.

2.3. Chemical Processes

The chemical processes represented in REMSAD represent several different categories including gas-phase, aqueous phase, aerosols, toxics, and mercury. A discussion of how each of these is represented in REMSAD follows. For reference to the following discussion, the species simulated by the REMSAD model are listed in Table 2-1. This list includes all gaseous, particulate, and toxic species.

Table 2-1
REMSAD Output Species

REMSAD Species	Description	Molecular Weight
NO	Nitric oxide	30
NO2	Nitrogen dioxide	46
O3	Ozone	48
CARB	Carbonyl	30
VOC	Volatile organic compounds (See note 1.)	16
NO2S	NOx mass accounting species	46
PNA	Peroxy nitric acid	79
PAN	Peroxyacetyl nitrate	121
CO	Carbon monoxide	28
HNO2	Nitrous acid	47
H2O2	Hydrogen peroxide	34
HNO3	Nitric acid	63
NTR	Organic nitrate	77
SO2	Sulfur dioxide	64
SULF	Sulfuric acid	98
ISOP	Isoprene	80
TERP	Monoterpenes	160
NH3	Ammonia	17
NAPH	Naphthalene	128
POM1	Polycyclic organic matter	178
POM2	Polycyclic organic matter	252
HG0-n	Elemental mercury (See note 2.)	201
HG2-n	Gaseous divalent mercury	201
DIOXIN	Gaseous Dioxin	322
ATRAZ	Atrazine	216
PNO3	Particulate nitrate	62
POA	Primary organic aerosols	1
PEC	Primary elemental carbon	1
ASO4	Aqueous pathway sulfate particles	96
GSO4	Gaseous pathway sulfate particles	96
NH4S	Ammonium associated with sulfate	18
NH4N	Ammonium associated with nitrate	18
SV1	Less volatile class of semi-volatile anthropogenic organic product species	136
SV2	More volatile class of semi-volatile anthropogenic organic product species s	136
SV3	Less volatile class of semi-volatile biogenic organic product species	168
SV4	More volatile class of semi-volatile biogenic organic product species	168
SOA1	Secondary organic aerosols from the SV1 class of compounds	136
SOA2	Secondary organic aerosols from the SV2 class of compounds	136
SOA3	Secondary organic aerosols from the SV3 class of compounds	168
SOA4	Secondary organic aerosols from the SV4 class of compounds	168
PMFINE	Primary fine particulate matter PMFINE $\leq$ 2.5 μm (See note 3.)	1

REMSAD Species	Description	Molecular Weight
PMCOARS	Primary coarse particulate matter 2.5 μm $\leq$ PMCOARS $\leq$ 10 μm	1
HG2P-n	Particulate divalent mercury	201
CD-n	Cadmium	112
POM1P	Particulate polycyclic organic matter	178
POM2P	Particulate polycyclic organic matter	252
DIOXP	Particulate dioxin	322
ATRAZP	Particulate atrazine	216

Notes:

1. TOL and XYL may be included in the emissions file, but are not simulated by the model. These species are used to calculate the aromatic fraction in the emissions. For further information, see the section on SOA.

2. Multiple Hg and Cd species are included to allow tagging. "-n" can range from 1 to 24 for Hg species and 1 to 10 for Cd.

3. PMFINE here represents primary particulate emissions of crustal matter, soil, and other sources and should not be confused with the broader use of the term PM$_{fine}$ referring to all sources of fine particulate matter.

2.3.1. Gas-Phase Chemistry

There are two options available in REMSAD for the simulation of gas-phase chemical processes. The CB-IV micro-mechanism provides the more complete representation of photochemistry, photolysis, and oxidation processes and is therefore recommended for most REMSAD applications. The original parameterized approach to gas-phase chemistry, however, is maintained as part of the REMSAD code.

2.3.1.1. Carbon-Bond IV Micro-Mechanism

The photochemical mechanism module used in REMSAD is a reduced-form version of the Carbon Bond Mechanism - version 4 (CB-IV) (Gery et al., 1989) as enhanced to include radical-radical termination reactions. This reduced-form version is termed "micro-CB-IV" (μCB-IV) and is based on a drastic reduction in the speciation of the organic compounds; the inorganic and radical parts of the mechanism are identical to CB-IV. In the current implementation of micro-CB-IV in REMSAD there are three organic species. VOC represents the emissions of most anthropogenic species. The species CARB represents carbonyl species and is both emitted from anthropogenic sources and formed as a product of VOC reactions. An additional primary organic species representing biogenic emissions is also included, with kinetic characteristics representing isoprene. Simulation of gas phase chemistry with this limited set of organic species is feasible since the intent of the micro-CB-IV mechanism is not to predict ozone levels with the precision usually sought in air quality models designed to address the ozone issue *per se*. Rather, the mechanism in REMSAD provides a physically faithful representation of the linkages between emissions of ozone and PM precursors; the oxidizing capacity of the troposphere, represented primarily by the concentrations of radicals and hydrogen peroxide; and the rate of oxidation of the nitrogen oxide (NO_x) and sulfur dioxide (SO_2) PM precursors.

The design of this new treatment has focused on the fastest possible computer coding which might preserve, on the one hand, an accurate rendition of the volatile organic compound (VOC) and nitrogen oxide (NO_x) control strategies as predicted by the CB-IV mechanism, while on the other hand, still be capable of predicting virtually all the potential precursors to secondary particulate formation that involve gas-phase photochemistry. These precursors include intermediate free radicals such as the hydroxyl (OH), hydroperoxyl (HO_2), organic peroxyl

(RO$_2$), and nitrate (NO$_3$). Product species (and their reactions) such as hydrogen peroxide, nitric acid, and organic nitrates along with gas-phase conversion of sulfur dioxide (SO$_2$) have also been retained. The full CB-IV has been the standard of performance comparison for accuracy and computer efficiency.

Figures 2-2 and 2-3 show isopleth diagrams derived from box model simulations using the original CBM-IV and the reduced "micro" version. On these figures, the x-axis is ppb of VOC and the y-axis is ppb of NOx. Contour lines of maximum ozone are displayed. Figure 2-4 shows the differences between the results shown in Figures 2-2 and 2-3. These isopleth diagrams were generated using the OZIPM4 code (Gery and Hogo, 1988) that was developed for use with the EPA Empirical Kinetics Modeling Approach (EKMA) for ozone control strategy estimates, which uses a moving-box model. As can be seen in Figure 2-4, the differences between the original full chemistry and the special reduced reaction set or "micro" version are generally less than 5 percent.

In the implementation of micro-CB in version 7 of REMSAD (Table 2-2), the number of reactions is only reduced to 77 from the original reaction set of 86 reactions. Some of the current 77 reactions represent an expansion of the original set of CB-IV reactions. For instance, reactions have been added to treat low temperature conditions not normally treated by CB-IV. Additional reactions have also been added for the TERP species used in the SOA treatment. However, the number of organic "state" species carried in the model for the standpoint of emissions and transport has been reduced from a typical grid model value of 10 to only 2 (VOC and CARB). The number of radical species that are typically estimated in grid models using the steady-state approximation, however, is nearly unchanged. Grid model computer burdens are typically related to the number of "state" species simulated and not the number of species treated in steady-state. Recent advances in fast-solver integration schemes for computing the photochemical differential equations have been alleviating the computer burden of solving the matrix of equations defining the gas phase chemical transformations. With this new reduced reaction set for the photochemistry, not only can the computer cost be further reduced for integration of the chemistry, the emissions and transport computer costs can be reduced as well because the overall number of state species is reduced by approximately a factor of 2.

Version 7 of REMSAD includes several updates to the micro-CB relative to earlier versions of REMSAD. One of the most important updates is the treatment of the species NO3 and N2O5. These species are normally calculated in steady-state in CB-IV, but in UAM applications of the full carbon bond IV mechanism an additional species called NXOY has been used to ensure that nitrogen mass is conserved when NO2 and N2O5 concentrations increase at night. The NXOY species was not implemented in the fast solver version of micro-CB because the NXOY treatment was not readily compatible with the automated code generation system used to implement the fast solver. It later became apparent that nitrogen mass inconsistencies could occur in the solver without the presence of NXOY. Therefore, in the version of micro-CB implemented in Version 7 of REMSAD a new treatment for the NO3 and N2O5 species has been implemented that is compatible with the automated code generation system and is in some ways superior to the NXOY treatment.

In order to implement the new treatment, the species NO2 was renamed to NO2S. A new species NO2 was defined that is the sum of NO2S + NO3 +2*N2O5. (Note that in preparing inputs such as emissions or boundary concentration files, the user need not set NO2S. Set NO2 as usual and NO2S will be set automatically within the model.) NO2 was explicitly written into the reactions of the chemical mechanism as a product species. The mass of nitrogen-related species is therefore accounted for in NO2 regardless of how the mass is distributed between NO2S, NO3 and N2O5. Calculation of the concentrations of NO3 and N2O5 are made

by apportioning the mass represented by the difference of NO2 and NO2S. The NXOY species was used similarly. The incorporation of this change resulted in a more realistic fraction of nitrogen mass appearing as NO3 and N2O5. The quasi-steady-state calculation of NO3 and N2O5 is still possible when the reactions governing their formation are fast (i.e., during the daytime).

Two conditions are required in the model code for the quasi-steady-state calculation to be allowed: the calculated quasi-steady-state concentrations of NO3 and N2O5 must account for less than 1% of the mass of NO2S; and the residual mass of nitrogen represented by NO2 minus NO2S must be less than 1% of the NO2S mass. Using this new treatment results in improved agreement with rigorous solvers such as the Gear solver and eliminates the nitrogen mass inconsistencies noted earlier.

Several new reactions have been included in the updated version of micro-CB. These reactions are as follows: OH reacting with hydrogen (#14 in Table 2-2, using HO2 as a product) and OH reacting with NO3 (#20 in Table 2-2), and the HO2 reaction with NO3 (#21 in Table 2-2). These reactions are important because of the wide range of temperatures, pressures, and pollutant loadings that are used in REMSAD compared to the summer, ground-level, urban ozone conditions for which the full CB-IV has been used. These reactions have also been added to a new full Carbon Bond version (to be called CB-V). These reactions were added partly due to the work of Liang and Jacobson (2000) who compared the organic part of CB-IV against a 4,000-reaction mechanism used in European modeling. The inorganic reaction set used by Jacobson had most of these reactions added to those used in the original CB-IV. The European 4,000 reaction mechanism and the CB-IV were compared using the same updated and expanded inorganic reaction set and both total mechanisms for the most part were shown to give similar results when used to simulate urban smog episodes.

In addition to the above reactions the original reactions for peroxy nitric acid (PNA) recommended by Gery et al. (1989) were included, along with a reaction for the photolysis of PNA. These were added for the same reasons stated above. Under summer smog-like conditions the PNA reactions are not important and are not normally used in UAM applications of the full CB-IV mechanism but could be important in a continental scale simulation given the wide range of temperature, pressure, and concentrations encountered.

The reactions in Table 2-2 represent gas phase reactions and only the reaction of SO2 with the OH radical to form sulfate directly affects particulate concentrations. However, a number of the gas phase species affect the production of particulate in aqueous phase. Peroxide, which is a product of the gas phase chemistry, is important in the aqueous production of sulfate. To a lesser degree, ozone also affects the production of sulfate in aqueous phase. Nitric acid produced in gas phase can later be converted to particulate via reaction with ammonia. Radical species such as OH and HO2 can affect the evolution of toxics such as POM and mercury. The gas phase products (ozone, peroxide, nitric acid, and radicals) are the result of a complex interaction of many reactions in the mechanism. Secondary organic aerosol (SOA) is also a known product of gas phase interactions. Version 7 of REMSAD includes production of SOA through the gas phase chemistry, as discussed in more detail later in this section.

Table 2-2.
Micro-CB-IV reduced reaction set.

	REACTION	RATE CONSTANT (ppm^{-1}-min^{-1})	TEM. DEP. (K)
1	NO2S = NO + O - NO2	1.00E+00	0
2	O = O3	4.32E+06	-1175
3	O3+ NO = NO2S + NO2	2.66E+01	1370
4	O+ NO2S = NO - NO2	1.38E+04	0
5	O+ NO2S = NO3	2.31E+03	-687
6	O+ NO = NO2S+ NO2	2.44E+03	-602
7	NO2S+ O3 = NO3	4.73E-02	2450
8	O3 = O	1.00E+00	0
9	O3 = O1D	1.00E+00	0
10	O1D = O	4.25E+10	-390
11	O1D+ H2O = 2.0000 OH	3.26E+05	0
12	O3+ OH = HO2	1.00E+02	940
13	O3+ HO2 = OH	3.00E+00	580
14	OH+ HO2 =	1.63E+05	-250
15	OH = HO2	5.90E+00	2000
16	NO3 = 0.8900 NO2S+ 0.8900 O+ 0.1100 NO -0.1100 NO2	1.00E+00	0
17	NO3+ NO = 2.0000 NO2S + NO2	4.42E+04	-250
18	NO3+ NO2S = NO + NO2S - NO2	5.90E-01	1230
19	NO3+ NO2S = N2O5	1.85E+03	-256
20	NO3+ NO3 = 2.0000 NO2S	3.40E-01	2450
21	NO3+ OH = NO2S + HO2	3.25E+04	0
22	NO3+ HO2 = HNO3 - NO2	5.17E+03	0
23	N2O5+ H2O = 2.0000 HNO3 -2.0000 NO2	1.90E-06	0
24	N2O5 = NO3 + NO2S	2.78E+00	10897
25	NO+ NO = 2.0000 NO2S 2.0000 NO2	1.54E-04	-530
26	NO+ NO2S+ H2O = 2.0000 HNO2 - NO2	1.60E-08	0
27	NO+ OH = HNO2	9.80E+03	-806
28	HNO2 = NO + OH	1.00E+00	0
29	OH+ HNO2 = NO2S + NO2	9.77E+03	0
30	HNO2+ HNO2 = NO + NO2S + NO2	1.50E-05	0
31	NO2S+ OH = HNO3 - NO2	1.68E+04	-713
32	HO2+ NO2S = PNA - NO2	2.04E+03	-323
33	PNA = NO2S + HO2 + NO2	5.18E+00	10577
34	OH+ PNA = H2O2 + NO3+ NO2	6.80E+03	-380
35	PNA = 0.3900 OH+ 0.3900 NO3+ 0.6100 NO2S+ 0.6100 HO2+ NO2	1.00E+00	0
36	OH+ HNO3 = NO3+ NO2	2.18E+02	-1000
37	HO2+ NO = OH + NO2S+ NO2	1.23E+04	-240
38	XO2+ NO = NO2S+ NO2	1.20E+04	0
39	XO2N+ NO = NTR	1.20E+04	0
40	XO2+ XO2 =	2.00E+03	-1300
41	HO2+ HO2 = H2O2	4.14E+03	-1150
42	HO2+ HO2+ H2O = H2O2	2.18E-01	-5800
43	H2O2 = 2.0000 OH	1.00E+00	0
44	OH+ H2O2 = HO2	2.52E+03	187
45	OH+ CO = HO2	3.22E+02	0

	REACTION	RATE CONSTANT $(ppm^{-1}\text{-}min^{-1})$	TEM. DEP. (K)
46	CARB+ OH = 0.3000 HO2+ 0.3000 CO+ 0.7000 C2O3	1.30E+04	0
47	CARB = 2.0000 HO2 + CO	7.00E-01	0
48	CARB = CO	5.00E-01	0
49	CARB+ O = OH + HO2+ CO	2.95E+02	1550
50	CARB+ NO3 = HNO3 + HO2+ CO -NO2	1.60E+00	0
51	C2O3+ NO = CARB + NO2S+ HO2+ XO2+ NO2	2.82E+04	180
52	C2O3+ NO2S = PAN - NO2	1.37E+04	-380
53	PAN = C2O3+ NO2S+ NO2	2.54E-02	13500
54	C2O3+ C2O3 = 2.0000 CARB+ 2.0000 XO2+ 2.0000 HO2	3.70E+03	0
55	C2O3+ HO2 = 0.7900 CARB+ 0.7900 XO2+ 0.7900 HO2+ 0.7900 OH	9.60E+03	0
56	XO2+ HO2 =	8.90E+03	-1300
57	OH = CARB+ XO2+ HO2	2.10E+01	1710
58	VOC+ OH = 0.9000 XO2+ 0.1000 XO2N+ 0.2500 HO2 + 0.4000 ROR+ 0.8000 CARB+ 0.0800 C2O3 + a_1 SV1 + a_2 SV2	2.46E+03	0
59	ROR = 0.9600 XO2+ 0.0400 XO2N+ 0.9400 HO2 + 0.0200 ROR+ 1.1000 CARB	1.37E+05	8000
60	ROR = HO2	9.54E+04	0
61	ROR+ NO2S = NTR - NO2	2.20E+04	0
62	VOC+ O3 = CARB+ 0.4000 CO+ 0.3000 HO2 + 0.1000 XO2+ 0.0500 OH	4.00E-05	0
63	VOC+ NO3 = NO2S + XO2+ CARB	2.10E-01	0
64	VOC+ O = CARB+ HO2+ 0.5000 XO2 + 0.5000 CO	1.33E+02	0
65	OH+ SO2 = SULF + HO2	1.11E+03	-160
66	XO2N+ HO2 =	8.90E+03	-1300
67	XO2N+ XO2N =	2.00E+03	-1300
68	XO2N+ XO2 =	4.00E+03	-1300
69	ISOP+ O = 0.2500 HO2+ 0.2500 XO2+ 0.2500 C2O3 + 1.2500 CARB+ 2.5000 VOC	5.32E+04	0
70	ISOP+ OH = 1.5400 CARB + XO2+ 0.9100 HO2 + 0.0900 XO2N+ 2.7400 VOC	1.48E+05	-407.6
71	ISOP+ O3 = 1.4000 CARB+ 0.2000 C2O3+ 2.4500 VOC + 0.2660 OH+ 0.2000 XO2+ 0.0660 HO2+ 0.0660 CO	1.90E-02	1912
72	ISOP+ NO3 = CARB + XO2+ 0.8000 HO2 + 0.2000 NO2S+ 3.8000 VOC + 0.8000 NTR -0.8000 NO2	9.96E+02	448
73	ISOP+ NO2S = CARB + XO2+ 0.8000 HO2 + 0.2000 NO+ 3.8000 VOC + 0.8000 NTR - NO2	2.20E-04	0
74	TERP + O = 0.1470 CARB + 5.3000 VOC + $a_{3,1}$ SV3 + $a_{4,1}$ SV4	5.268E+04	0
75	TERP + OH = 0.7500 CARB + 1.2500 XO2 + 0.7500 HO2 + 0.2500 XO2N + 2.1000 VOC + $a_{3,2}$ SV3 + $a_{4,2}$ SV4	9.924E+04	-449
76	TERP + O3 = 0.4410 CARB + 0.7600 XO2 + 0.0650 HO2 + 0.1800 XO2N + 7.0000 VOC + 0.3860 C2O3 + 0.0010 CO + 0.5670 OH + $a_{3,3}$ SV3 + $a_{4,3}$ SV4	1.1E-01	821
77	TERP + NO3 = 0.4740 CARB + 1.0260 XO2 + 0.2760 HO2 + 0.2500 XO2N + 0.5000 VOC + 0.2760 NTR + 0.4740 NO2S - 0.5260 NO2 + $a_{3,4}$ SV3 + $a_{4,4}$ SV4	9.82E+03	-175

Figure 2-2

Standard CBM-IV as used in UAM

Figure 2-3

Micro CB Mechanism

Figure 2-4

Micro Mechanism minus standard CBM as used in UAM
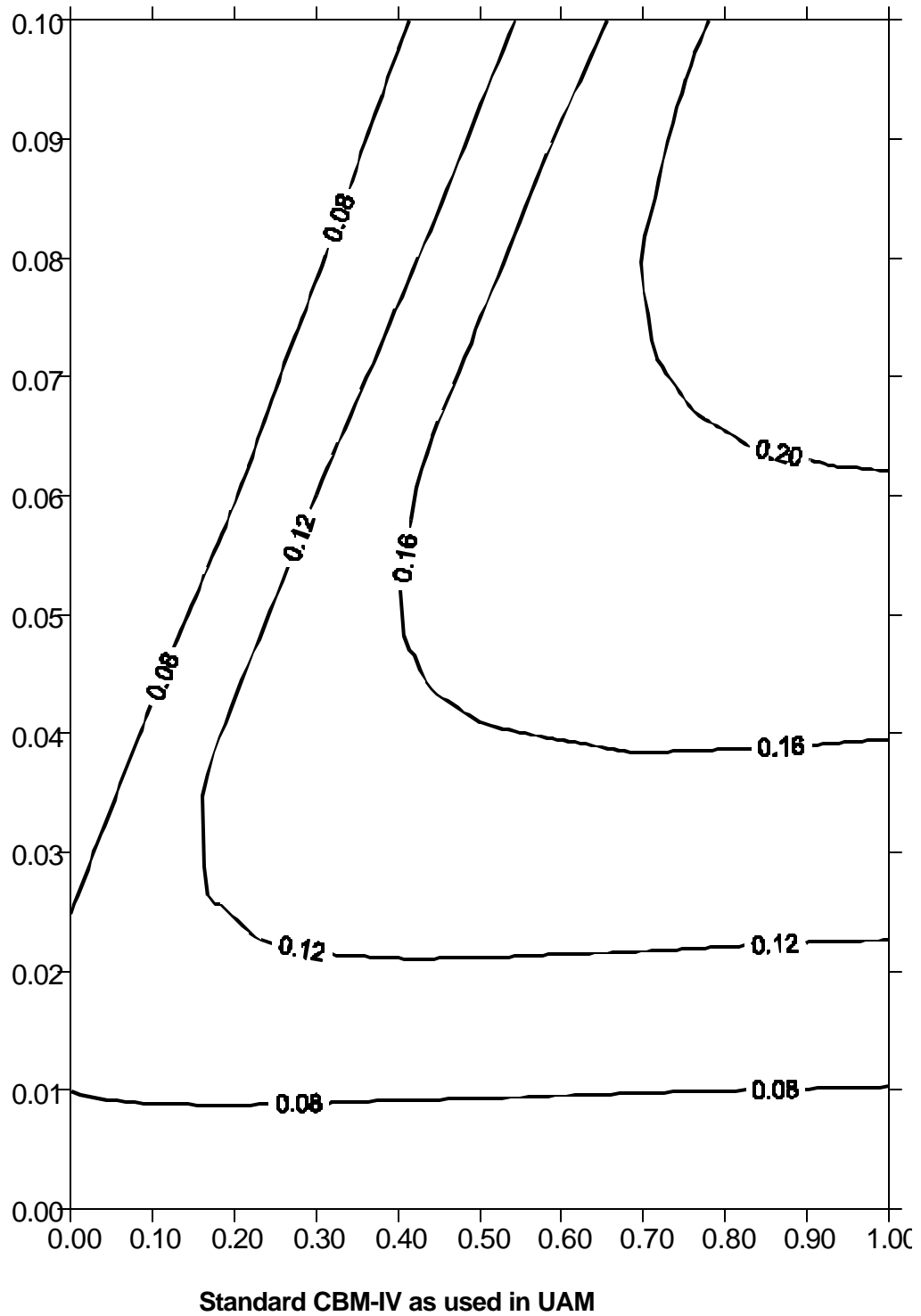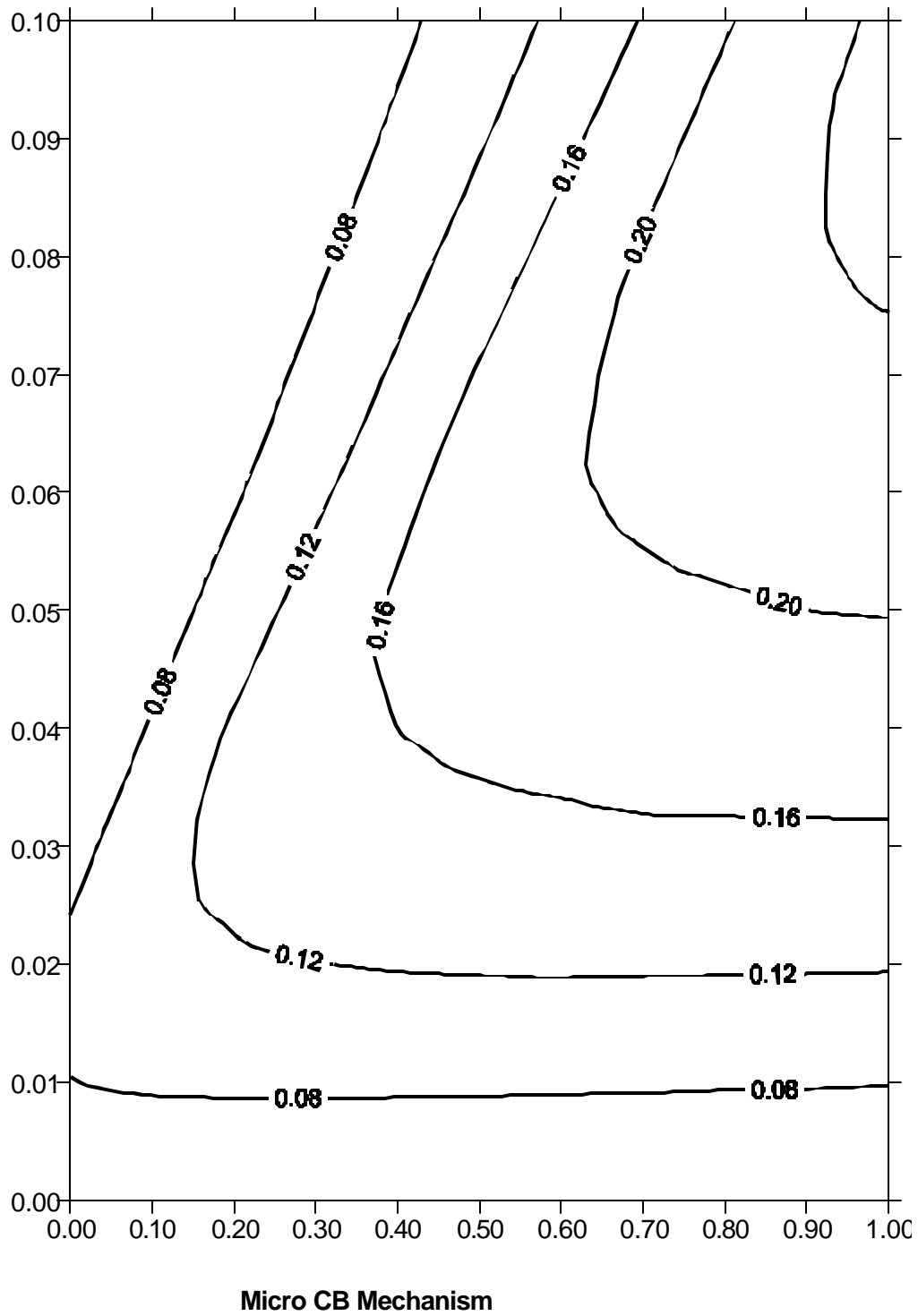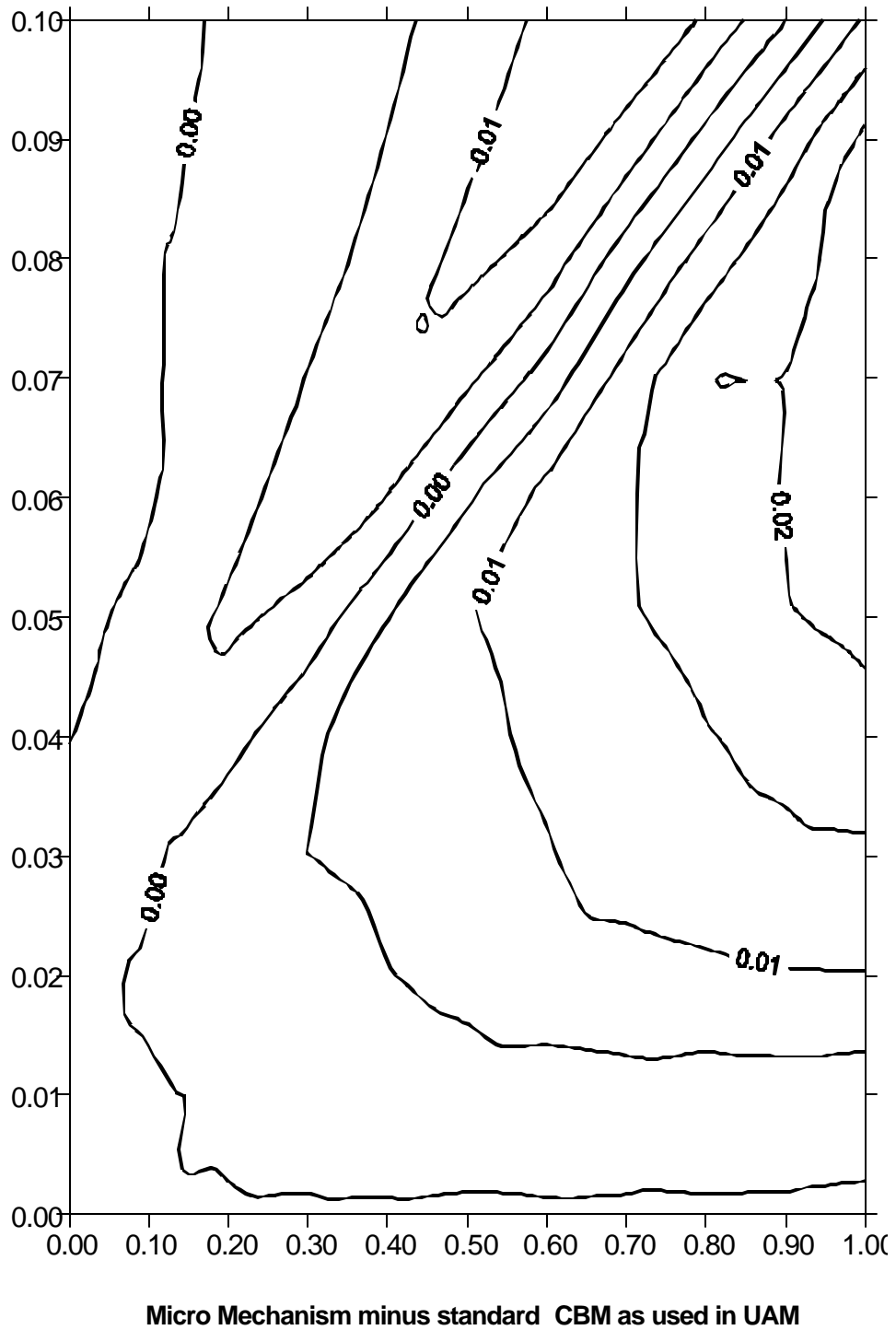
2.3.1.2.   Parameterized Gas-Phase Reactions

The second option for REMSAD is to use a parameterized set of reactions for the gas-phase chemistry. This approach provides the necessary fields of atmospheric oxidants (ozone and hydroxyl radical) for calculation of atmospheric particulates. The basis for the parameterized chemistry module is described by Gray et al. (1993). This approach incorporates the parameterized plume chemistry from the Regional Impacts on Visibility and Acid Deposition (RIVAD) Lagrangian plume segment model. Since RIVAD was originally developed for plume modeling, several modifications to the RIVAD chemistry were made in adapting it for use in a regional model. Use of the parameterized reaction is somewhat more computationally efficient than use of the micro mechanism, but the use of the micro mechanism is the recommended approach. Using this approach, ozone is an input variable and a total of five other gas phase species (NO_x, SO_2, NH_3, VOC, and nitric acid) are accommodated.

The parameterization scheme provides a first approximation to the photochemistry of importance for PM calculations. The parameterization accommodates a response in the hydroxyl radical (OH) concentration to changes in ozone, NO_x and light levels. The parameterization accounts for loss of hydroxyl by reactions with methane and carbon monoxide, and includes the effects of reactions of hydroxyl with NO_2, SO_2, and a single generic VOC species.

2.3.1.3.   Photolysis Rates

REMSAD requires information on solar radiation in order to calculate photolysis rates for the photochemical reactions that drive the formation of OH radical and to compute the steady-state concentrations of NO, NO2, and O3.

Photolysis rates are computed by a preprocessor that incorporates a parameterized light model developed by Schippnick and Green (1982). As a result, lookup tables for the NO2 and O3 photolysis rates were generated for various zenith angles and altitudes. From this table, ATDM calculates the photolysis rates on a cell-by-cell basis by linear interpolation between the nearest values of solar zenith angle and altitude.

The ratios of ozone, formaldehyde and acetaldehyde to NO2 photolysis rate have been defined for two altitudes (1380 m and 10000 m) that approximately represent the average altitude of the boundary layer and the upper troposphere. These ratios as well as O3 photolysis rates were used to generate OH lookup tables for the lower and upper atmospheres. Photolysis rates for several other photochemical reactions are derived from these values using scaling factors (see Gery et al., 1988).

Cloud cover is not treated by the photolysis rate preprocessor, but at the end of each time step all photolysis rates are corrected for cloud cover using the algorithm developed by Chang (1987) for RADM. The cloud cover scaling factors applied to the photolysis rates vary from 1 for clear skies to 0.01 for completely overcast conditions (under some cloud vertical distribution this scaling factor can be higher than 1). Attenuation factors for other J values may be different, although there is no information on the attenuation of photolysis rates for chemicals other than NO2. Thus, as a first approximation we assume that the cloud cover effects for all photolysis rates are the same as for NO2.

2.3.2.   Aqueous-Phase Sulfate Chemistry

Chemical processes that occur in the aqueous phase (clouds, rain, and fog conditions) can be important in the formation of secondary particulate matter and in the transformation of toxic pollutants. The aqueous-phase chemical process of primary importance for PM applications in REMSAD is sulfate formation. Aqueous-phase (or in-cloud) processes can account for the majority of atmospheric sulfate formation, especially in the wintertime when gas-phase chemistry is slow.

Three important pathways for in-cloud sulfate formation are treated in REMSAD: (1) the reaction of aqueous SO_2 with ozone, (2) the reaction of aqueous SO2 with molecular oxygen (catalyzed by iron and manganese), and (3) the reaction of aqueous SO_2 with hydrogen peroxide (H_2O_2). For pH levels below about 4. (a common situation in the eastern U.S), the ozone and oxygen reactions are slow and the H_2O_2 reaction dominates. Therefore, versions of REMSAD prior to version 7 included only the H2O2-SO2 reaction in the cloud chemistry. However, to include potential contributions to sulfate formation of the other two reactions, REMSAD has been updated to include aqueous reaction of SO2 with ozone and oxygen. REMSAD currently has no internal estimation of cloud pH and utilizes a constant value of 4.5. Therefore, the H2O2-SO2 reaction pathway is still expected to dominate, but the addition of the other reactions allows their contribution to be incorporated. If a variable pH is implemented in REMSAD, it is straightforward to adapt the current treatment to the variation in the rates due to variation in pH.

H_2O_2 is often present at the ambient concentrations below those of SO_2. Thus formation of sulfate can be limited by the availability of H_2O_2. It can also be quite nonlinear. The formation of H_2O_2 is tied to the overall atmospheric photochemical system, and responds to changes in ambient levels of VOC and NO_x. Because of this link, emission changes for VOC and NO_x may have effects on ambient sulfate levels that are equal to or greater than effects due to changes in SO_2 emissions.

There are two versions of sulfate chemistry available in REMSAD. When the micro-CB-IV chemical mechanism is selected, the aqueous reactions of SO_2 with peroxide, ozone, and oxygen are used directly to estimate the rate of sulfate formation. A formulation for representing the aqueous SO2 reactions is presented by Martin (1984; 1994). By taking the following equation from Martin (1984) for the rate of change of SO2 due to reaction with a soluble gas, the rate of change of SO2, ozone and H2O2 due to all three reactions can be calculated. The form of all three reactions is the same. Martin gives

$$d(SVI)/dt = k \, (K_{Hs} * SO2) * (K_{Hr} * C_r) * LWC$$

where SO2 is the partial pressure of SO2, Cr is the partial pressure of the reactant (H2O2, O3, or O2), K_{Hs} is the effective Henry's law coefficient for SO2, K_{Hr} is the effective Henry's law coefficient for the reacting gas (H2O2, O3, or O2), k is the reaction rate, and LWC is the liquid water content. D(SVI)/dt is the formation rate of sulfate. The negative of this value gives the destruction rate of SO2 and for the reacting species (H2O2, O3, or O2). The concentration of O2 is assumed to remain constant during the calculation of the amount of sulfate formed. A value of 4.6×10^6 $M^{-1}sec^{-1}$ was estimated for k for the SO2-ozone reaction from figure 28 of Martin (1994). From Figure 21 in Martin (1984), a value of 2.3×10^3 $M^{-1}sec^{-1}$ was estimated for k for the H2O2 reaction. The O2 reaction can cover a broad range of reaction rates depending on the amount of iron and manganese in solution. Following Martin (1994), iron and manganese are assumed to be present at concentrations of approximately 3×10^{-7} M and 3×10^{-8} M respectively.   A rate of 3.2 $M^{-1}sec^{-1}$ for k in the O2 reaction results in an hourly conversion rate

that is consistent with this assumption and that falls in the range shown in Figure 30 of Martin (1994).

Cloud liquid water content is an input to REMSAD and is expressed as volume mixing ratio (LWC in the above equation) for use in these rate calculations. Low liquid water content would therefore inhibit the progress of the reactions. All three reactions would be affected in the same way by changes in liquid water content.

A simple finite differencing calculation can calculate the resulting concentrations of SO2, O3 and H2O2 after one REMSAD time step. Partial pressure of oxygen is assumed to remain constant. During this calculation, the average amount of dissolved SO2 is saved for later use in the mercury chemistry calculations.

Sulfate formation in parameterized form

When the parameterized chemistry is specified, a parameterized in-cloud sulfate formation algorithm is used. The parameterized in-cloud sulfate formation algorithm is adopted from the RTM-II model (ref). In this algorithm, relative humidity is used as surrogate for clouds. The humidity-dependent heterogeneous SO_2 conversion rate (R_{SO2}) is calculated from the following formula:

$$R_{SO2} = \exp [0.072 (RH - 70)] -1 \ (\%/hr)$$

where RH is relative humidity. This equation was developed based upon measured SO_2 conversion rates for power plant plume in the literature (Dittenhoefer and De Pena, 1980). The equation is only applied when RH exceeds 70 percent. The highest RH value is capped at 95 percent, resulting in a maximum SO2 conversion rate of 5 percent per hour. (The typical gas-phase conversion rate is 1 percent per hour). This parameterized estimation of sulfate formation is only used when the parameterized chemistry option is specified. The use of the micro mechanism and the aqueous sulfate chemistry module is recommended.

2.3.3.   Aerosols

2.3.3.1.   MARS-A Equilibrium Scheme

Secondary particulate matter is formed in the atmosphere through the oxidation of emitted NOx and SOx to form sulfate and nitrate species. In REMSAD, all sulfate is assumed to be in aerosol phase. The species GSO4 in REMSAD tracks the sulfate formed via gas phase chemical reactions (see the section on gas phase chemistry above). ASO4 tracks the sulfate formed via aqueous reaction pathways (see aqueous chemistry, above). The species SULF is a product species of the SO2 + OH reaction in the gas phase chemistry. During each time step the incremental increase in SULF during the gas phase chemistry is calculated and added to GSO4, which represents sulfate formed from gas phase processes. GSO4 is then used in any further analyses of the sulfate from gas phase. During post-processing, ASO4 and GSO4 are typically added together to get TSO4, the total amount of particulate sulfate.

Another source of secondary PM is nitrate. The calculation of the contribution of nitrate to PM is more complex than for sulfate due to the interaction of sulfate, nitrate, and ammonia. The species sulfuric acid, nitric acid, ammonium nitrate, and ammonium sulfate reach an equilibrium that is a function of the relative amounts of nitrate, sulfate and ammonia and local meteorological conditions. Prior versions of REMSAD used a parameterized chemistry to calculate this equilibrium state. In version 7, the MARS-A algorithm as developed for the EPA's MODELS-3 system has been implemented in REMSAD.

The MARS-A routine takes as input the total ammonia, total nitrate and total sulfate. As implemented in REMSAD, the MARS-A routine is used to determine the amounts of nitric acid, particulate nitrate, and ammonia in the form of ammonium nitrate and in the form of ammonium sulfate. The methodology used in MARS-A is documented by Saxena (Saxena et al., 1986) and by Kim (Kim et al., 1993). In this section, the use of MARS-A in REMSAD is discussed in general terms. For further detail on MARS-A, the reader is referred to the aforementioned papers.

MARS-A breaks the calculation into several different regimes. The first major break is between an ammonia rich environment (total ammonia more than twice sulfate, on a molar basis) vs. an ammonia deficient environment. The ammonia rich regime is further broken down based on the mass fraction of liquid water (diagnosed within MARS-A). One case is below the deliquescence point of ammonium nitrate (RH approximately 62%). In this low humidity regime particulate ammonium nitrate can form through an equilibrium of gas phase nitric acid and ammonia. For higher humidity, formation of ammonium nitrate in aqueous phase is considered. This calculation is further broken down by considering cases above and below the deliquescence point of ammonium sulfate (80%). MARS-A determines an aqueous equilibrium fraction of ammonium nitrate with ammonium sulfate supersaturated.

In the ammonia deficient case, MARS-A considers ionic strengths of hydrogen ion and sulfate compounds in aqueous solution in order to determine the solubility of nitrate. MARS-A considers the ratio of the ammonia to sulfate concentration and up to 6 different compounds ($(NH_4)_2SO_4$, H_2SO_4, NH_4HSO_4, $(NH_4)_3H(SO_4)_2$, NH_4NO_3, and HNO_3) in this regime in determining the ammonium nitrate concentrations. This detailed treatment is in contrast to the earlier implementation in REMSAD, which used a simple interpolation between no ammonium nitrate and the ammonia rich case. In particular, MARS-A allows for the possibility of the presence of ammonium nitrate even when total ammonia is less than total sulfate.

Implementation of MARS-A in REMSAD required developing a driver routine to replace the *eql* routine in the original module obtained from the Community Multi-scale Air Quality (CMAQ) model. This driver passes required concentration and meteorological data to the *rpmares* routine, which then calculates the equilibrium concentrations. Modifications to *rpmares* were quite limited and were only what was required in order to provide concentration and meteorological data from the REMSAD data arrays rather than the CMAQ model arrays. In the REMSAD core model (ATDM), the calls to the *nitrat* routine were replaced with calls to the new driver routine, *remeql3*. Input data for the *remeql3* routine is concentration of total nitrate, total sulfate, total ammonia and total ammonium. The routine is also provided with local meteorological data. The routine returns concentration of nitrate that is in the form of nitric acid, the concentration of nitrate in particulate form (i.e., as ammonium nitrate), the concentration of free ammonia, and the concentration of ammonium sulfate.

The total nitrate supplied to the routine is the sum of HNO3 and PNO3. Total sulfate is calculated as the sum of ASO4 and GSO4, which represent, respectively, the sulfate produced from aqueous phase reactions and gas phase reactions. Total ammonia is the REMSAD species NH3. Total ammonium is the sum of the REMSAD species NH4N and NH4S.

Only the *rpmares* routine from the CMAQ aerosol package is used in REMSAD. Routines treating other processes, such as deposition, are not used in REMSAD since these processes are treated elsewhere in REMSAD.

2.3.3.2. *SOA Treatment*

Organic aerosols can contribute a significant amount to the PM in the atmosphere. Primary organic aerosols (POA) are treated as a directly emitted species in REMSAD. In REMSAD version 7, a calculation of the production of secondary organic aerosols (SOA) due to atmospheric chemistry processes has been added.

Treatment of SOA in prior versions of REMSAD consisted of adding a directly emitted SOA species to the emissions inventory. The amount of SOA in the inventory was based on VOC emission factors developed by Grosjean (1992) for the South Coast Air Basin, which reflect time scales that may not apply to the larger domain typically simulated by REMSAD. The REMSAD model should be able to reflect observed seasonality and regional differences in SOA. For example, SOA can be expected to be greater in summer because of higher oxidant levels, higher evaporative emissions, and higher biogenic emissions.

A peer review of the REMSAD model (Seigneur et al., 1999) recommended an SOA module based on the equilibrium approach of Pankow as is used by Odum et al. (1997) and Griffin et al. (1999). The implementation of the SOA treatment follows the recommendation of the peer review.

The SOA treatment includes SOA formation from anthropogenic and biogenic organic precursors. The REMSAD treatment includes gas phase species SV1 and SV2 with corresponding aerosol phase species SOA1 and SOA2 for the anthropogenic organics, and gas phase species SV3 and SV4 with corresponding aerosol species SOA3 and SOA4 for the biogenic organics. The separation of these two types of emissions in the gas phase chemistry and precursor emissions modules of the REMSAD model has made the separate calculation of anthropogenic and biogenic SOA possible. This separation is also appropriate because, as noted by Jacobson (1999), natural sources contribute more to particle loading (345-2080 Tg/yr SOA), but the relative contribution of anthropogenic (currently 140-396 Tg/yr) is typically increasing, and in urban regions anthropogenic sources may exceed natural sources.

Early attempts to represent SOA formation were primarily based on fractional aerosol coefficients (FAC), which were determined experimentally. However, a series of papers by Pankow (1994) and the experimental work of Odum et al. (1997) suggest that a significant departure from PM models using only empirical FAC treatments would be needed. For example, Odum et al. (1997) note that "observed SOA yields from a-pinene can range from less than 10% to greater than 50%. Pankow noted that once semi-volatile organics have begun to condense, a layer on existing particles appears to form such that some mass is partitioned onto this layer even though gas phase concentrations may still be below saturation. Moreover, this partitioning has been found to vary with the existing organic aerosol mass (M_0). Thus the amount of a semi-volatile organic compound that is present in the aerosol phase depends not only on the total amount of that particular compound in the atmosphere, but also on the amount of all organics that have already condensed to aerosol phase.

Odum et al. (1997) showed that the organic fraction of secondary PM2.5 attributable to gasoline in the atmosphere could be completely accounted for by just the aromatics content of the gasoline. That is, at least for the anthropogenic emissions, it may be possible to account for the resulting SOA by considering only the aromatics reactions.

The approach implemented in REMSAD is based on the papers cited above. The two papers by Odum et al. (1997) and Griffin et al. (1999) use a similar approach. The main focus of the

Odum et al. (1997) paper is on anthropogenic precursors in the California Institute of Technology (CIT) air quality modeling system; the focus of the paper by Griffin et al. (1999) is on biogenics. Here the discussion will follow similar lines by treating the anthropogenics first. In the existing REMSAD chemistry two species (VOC and CARB) are used for all anthropogenic VOC emissions. Aromatics are a fraction of the REMSAD VOC species.

Local differences in the aromatics fraction can be important to accurately simulate local SOA, but these local variances can be imbedded into the stoichiometric product fractions using a spatially (and possibly temporally) varying factor f_A that represents the local fraction of aromatics.

In the CIT model, only aromatics are used to simulate anthropogenic SOA. These consist of two types: TOLU (for toluene) and AROM (for higher aromatics). Two hypothetical condensable vapor products are assumed to yield from each of the reactions of aromatic compounds with the hydroxyl radical. For example,

$$AROM + OH = \dots + a_1 \, AAR1 + a_2 \, AAR2,$$
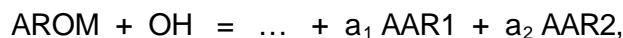
where a_1 and a_2 are stoichiometric coefficients. For REMSAD a similar treatment is used such that

$$VOC + OH = \dots + a_1 \, SV1 + a_2 \, SV2,$$

where SV1 and SV2 are the semi-volatile organic species produced and the a_1 and a_2 are similar to the coefficients used in the CIT model but reduced by the fraction of anthropogenic VOC that is aromatics as defined in the CIT model (i.e., $a_1 = a_1 \cdot f_A$). It should be noted that the CIT model uses two species for aromatics and the reduced Carbon Bond chemistry on which our SOA module is based uses only one. This approach appears to be a good approximation for simulation of SOA production. Based on analysis of experiments by Odum et al. (1997) the yield factors for SOA in REMSAD (that is, the values of a_1 and a_2) have been set to 0.05 and 0.162. The determination of f_A will be discussed below.

The Pankow mechanism as implemented in the CIT model is characterized as a gas/particle partitioning absorption mechanism. This type of model requires the use of a sorption partitioning constant K_i that implies that the amount of condensable species that is in the particulate phase is proportional to the organic aerosol mass concentration (M_0).

$$K_i = (P_i / M_0) / G_i$$

where G_i and P_i are the gas-phase and particle phase concentrations of the semi-volatile organic products formed from the VOC as noted above (e.g., SV1 and SV2). The values used by Odum et al. (1997) for K_2 were similar whether the SV2 product was produced from m-xylene or 1,2,4-trimethybenzene, but the K_1 values for the SV1 product differed depending on which reactant was considered (0.032 for m-xylene and 0.053 for the trimethylbenzene). For the REMSAD treatment, average values of K_1 and K_2 were developed based on the CIT experimental values and ambient averages for typical aromatics mixtures. The resulting values for K_1 and K_2 are 0.047 and 0.0016 respectively. The temperature dependence of the K values is implemented as $K_x(T) = K_x \, e^{10000 \, (1/T - 1/298)}$, where T is in degrees Kelvin. Recent work by Jang and others (Jang and Kamens, 1998; Jang et al., 1997) suggests that some SOA probably forms on existing aerosols other than organic aerosols. Data to establish partitioning coefficients for the formation of SOA on non-organic aerosols is, however, not yet available. We have therefore not included non-organic aerosols in the SOA partitioning formulation. The SOA

estimated by REMSAD could be considered a lower bound estimate of SOA since inclusion of non-organic aerosols in the partitioning would only serve to increase the SOA estimate.

For the anthropogenic SOA, REMSAD has two new gas phase species added, SV1 and SV2. The aerosol phase species corresponding to these are SOA1 and SOA2. The organic mass concentration, M_0, is calculated as the sum of primary organic aerosol (POA) and SOA (SOA in REMSAD is the sum of the particle fraction of all SVx species), with the fractions of SV1 and SV2 partitioned between the gas and particulate phases according to equilibrium constants K_1 and K_2 respectively. Finally, reaction of the SV2 species with the OH radical can result in conversion of SV2 to SV1. This reaction is implemented in REMSAD with a reaction rate of 1 X 10^4 ppm^{-1} min^{-1}.

The user has two options for setting the aromatic fraction, f_A. A default value of f_A is provided in the CHEMPARAM file, which will be used if a spatially and temporally varying fraction is not available. Currently the recommended value for this default is 0.33.

In order to set a spatially and temporally varying aromatic fraction, the user must provide additional information in the emissions file. In the Carbon Bond (CB) mechanism, aromatics are represented by the species TOL and XYL. The user should therefore include emissions of TOL and XYL in the emissions file, calculated using the standard CB speciation profiles. Note that it is not necessary to adjust the VOC and CARB emissions when TOL and XYL are included in the emissions files. REMSAD does not utilize the TOL and XYL emissions in calculating the gas phase chemistry. These species are used only to calculate f_A and are not advected or used in other aspects of the chemistry. If TOL and XYL do not appear in the emissions file, the default value of f_A will be used automatically.

Although TOL and XYL represent aromatic species, not all of the mass of aromatic compounds is accounted for in the mass of these species. Because aromatic compounds may include some parafinic or olefinic bonds, some of the aromatic mass is normally included in PAR or OLE. In order to estimate the amount of this additional aromatic mass, we utilized information from EPA's SPECIATE software (version 3.1). The SPECIATE software is used to develop VOC inventories and has one profile noted as "overall average." Assuming that this designation is a good one, we have used it to develop a correction factor to account for the additional mass.

Code 0000 in SPECIATE has a profile of 291 compounds listed by percent weight contribution. Of the 291 species, 38 are aromatic in nature that lead to some amount of TOL and XYL when processed in the EPS2 system. Some other aromatics are listed (e.g., benzene), but these are not treated by either TOL or XYL in the CB mechanism because their ozone-forming chemistry is significantly less important (and different) than aromatics that react like toluene (i.e., TOL). All such (low ozone importance) aromatics are assumed to be not important for secondary organic aerosol (SOA) formation. The steps used to estimate the additional aromatic mass follow.

- The profile for code 0000 was loaded into a spreadsheet.

- Each of the 38 important aromatic species was processed using the spreadsheet matrix used in EPS2 for converting compounds listed in the SPECIATE profiles into CB species.

- The units were then all converted to moles carbon using the known carbon numbers of the original species and the CB species.

- The sum contribution to each CB species was then added up for all 38 original aromatic species. The 38 aromatic species contributed mass only to the CB species OLE and

PAR in addition to TOL and XYL. A cross-check revealed that some carbon was treated as non-reactive.

- The sum of all 38 actual aromatics species (SumAro) was also obtained (in moles carbon).

- An equation was then set up such that a correction factor (Cf) multiplied times TOL plus XYL in moles carbon would equal SumAro. (i.e., Cf*(7*TOL + 8*XYL) = SumAro)

The value of Cf determined in this way was 1.18 with about half of the 18% correction being due to non-reactive treatment.

Version 7 of REMSAD calculates the aromatic fraction using the emissions of TOL, XYL, VOC, CARB and the factor Cf as:

$$f_A = Cf*(7*TOL + 8*XYL)/(VOC + CARB).$$

This calculation is made at each emissions update interval and in each grid cell. Note that the factor Cf is not applied to the default value of f_A that is provided by the user in the CHEMPARAM file.

For the biogenic SOA, a treatment similar to the anthropogenic treatment is implemented. In a recent paper Griffin et al. (1999) report experimental results useful to the methodology for SOA used in the CIT approach. Unlike anthropogenic VOC, which yield SOA mainly from aromatics reacting with OH, biogenics tend to be significantly reactive with nitrate radicals (NO3), free oxygen, and ozone as well as OH. In REMSAD, a condensed scheme for isoprene has been used to represent the ozone chemistry for all biogenics. The assumption that isoprene is a good surrogate for ozone chemistry is probably more valid than being a surrogate for SOA formation. In fact, isoprene has been shown by Pandis et al. (1991) not to produce SOA at atmospheric levels. In order to accurately represent the biogenic SOA formation in REMSAD, a new gas phase species, TERP representing monoterpenes, has been added. The addition of TERP has the side benefit of slightly improving the representation of the effects of biogenics on ozone chemistry. Thus, biogenic emissions in version 7 of REMSAD are now made up of ISOP and TERP emissions. For the biogenics two semi-volatile product species, SV3 and SV4, have been added. The reactions leading to biogenic SOA in REMSAD are therefore as follows:

$$TERP + OH = \ldots + a_{3,OH} SV3 + a_{4,OH} SV4,$$

$$TERP + O = \ldots + a_{3,O} SV3 + a_{4,O} SV4,$$

$$TERP + O3 = \ldots + a_{3,O3} SV3 + a_{4,O3} SV4,$$

$$TERP + NO3 = \ldots + a_{3,NO3} SV3 + a_{4,NO3} SV4.$$
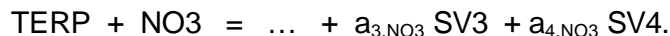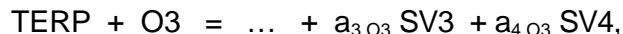
Partitioning coefficients, K_3 and K_4, are used with the partitioning formula described earlier for anthropogenic SOA in order to determine the fraction of SV3 and SV4, which condense to an aerosol state. Since K_3 and K_4 differ somewhat depending on which reaction resulted in the product, K_3 and K_4 are calculated at each time step as the weighted average of the amount of the product species produced by each of the four reactions. The temperature dependence of the K_3 and K_4 values is implemented in the same way as for the K_1 and K_2 values (see above). The values for a_3, a_4, K_3, and K_4 are based on average (non-isoprene) mixtures and the CIT experimentally determined values. The values are summarized below:

Reaction	a_3	a_4	K_3	K_4
TERP + OH	0.063304	0.324763	0.098145	0.003490
TERP + O	0.110681	0.417200	0.126386	0.004837
TERP + O3	0.109981	0.389277	0.142002	0.004704
TERP + NO3	0.092287	0.395069	0.125645	0.004385

Reaction of the SV4 species with OH can produce SV3. This reaction is implemented in REMSAD with a rate of 1×10^5 ppm^{-1} min^{-1}.

Since the SOA products will eventually be compared to observed data for SOA weight concentrations, it is necessary to assign appropriate molecular weights to these organic product species. The VOC species in REMSAD is treated as a single carbon species, but actually must represent hydrocarbons ranging from single carbon molecules to much more complex molecules. The semi-volatile products contain several carbon atoms. In addition, for each carbon in an SOA molecule there is additional mass from oxygen and other atoms in the molecule.

The commonly accepted molecular mass to carbon mass ratio of field SOA is about 1.4. Under controlled experimental conditions Yu et al. (1999) identified and measured the SOA products from the ozone reaction with a–pinene. For pinene 10 compounds were identified with mass to carbon ratios ranging from 1.4 to 1.79 and a standard error of 0.12. A yield-based analysis of these products results in an average mass to carbon ratio of 1.6. Kamens and Jaoui (2001) also measured and identified the species in SOA for a-pinene and their analysis confirms the results of Yu et al. (1999). The average carbon number for the SOA was 9.5 from both groups. Jang and Kamens (2001) identified the compounds in the SOA from toluene, but estimating a mass to carbon ratio from their work was more difficult as the relative amounts of the various products were not clearly delineated. For the 21 compounds that were identified in the toluene analysis, the range was 1.45 to 3.08 and the std. error was 0.39. A rough estimate gives a ratio of 1.9 for toluene with an average carbon number of 5.3. Although there is some evidence that higher values might be more appropriate, we have settled on using a mass to carbon ratio of 1.4, consistent with the field value, for both anthropogenic and biogenic SOA. Note that in the post-processing of the model output, these ratios can be changed. For carbon number, we have used 8.1 for anthropogenic (based on the average aromatic size) and 10 for biogenic SOA products. Therefore, the molecular weights assigned are 136 for SV1, SV2, SOA1, and SOA2, and 168 for SV3, SV4, SOA3, and SOA4.

Each of the species SV1, SV2, SV3 and SV4 is treated as a gas phase state species in REMSAD and is advected with other species. SV1, SV2, SV3 and SV4 have been assigned deposition properties similar to formic acid. The species SOA1, SOA2, SOA3, and SOA4, which replace the SOA species, are treated as particulate species in REMSAD. The deposition of these species is treated according to the standard REMSAD treatments for particulate matter.

2.3.4. Toxics

Chemical and physical process for five toxic species, mercury (Hg), cadmium (Cd), dioxin, polycyclic organic matter (POM), and atrazine (ATRAZ), are simulated by REMSAD. The

treatment for mercury is discussed in the following section of the user's guide; all others are briefly discussed here.

The atmospheric chemistry and physics (gas/particulate partitioning) are estimated based on the parameters available from the core chemistry module specifically ozone, OH, and particulate matter. Most of the toxic species in REMSAD are subject to one or both of two basic processes in addition to the usual transport and deposition processes: (1) oxidation via reaction with the OH radical; and (2) partitioning between the gas and particulate phases. Exceptions to this general rule are cadmium, which is treated as a particulate only species in REMSAD, and mercury, which is subject to a much more complex chemical treatment than the other toxic species.

2.3.4.1.   Cadmium

Cadmium (Cd) is involatile and therefore associated only with particulates. Cadmium is therefore treated as a single particulate species. (There is a tagging treatment available for cadmium; see discussion of tagging below.) No chemical reactions are included for cadmium. The emission, transport and deposition of Cd attached to particulate matter are treated as discussed in the following section on these model processes.

2.3.4.2.   Dioxins

Chlorinated dibenzodioxins and dibenzofurans (hereafter referred to generally as dioxins) are semi-volatile and exist in the atmosphere partially in the gas phase and partially associated with particles. The degree of association with particles increases with the degree of chlorination.

Available emissions data for dioxin are expressed as TEQ (toxicity equivalents). This is essentially a weighted average total dioxin measure in which 2,3,7,8-tetrachlorodibenzodioxin (the most toxic congener) is assigned a weighting factor of one, the 2,3,7,8-pentachlorodioxins and 2,3,4,7,8-pentachlorodibenzofuran are assigned a weighting factor of 0.5, 2,3,7,8-hexa-chlorodioxins and furans are assigned a weighting factor of 0.1, and other congeners have weighting factors less than 0.1. REMSAD uses a single dioxin congener with physical/chemical properties midway between those of the tetrachloro and pentachloro congeners. The REMSAD model tracks this congener as two species: a gas phase species and a particulate phase species. These species are partitioned between the gas and particulate phases as described below for POM species with sub-cooled liquid vapor pressure defined by

$$P_L(T) = 9\text{X}10^{-7}e^{7000(1/298\text{-}1/T)}, \text{ where } T \text{ is ambient temperature in K.}$$

Dioxins are somewhat reactive in the atmosphere. The higher chlorinated congeners undergo photolytic dechlorination, whereas the lower chlorinated congeners react with the OH radical. The tetra- and pentachloro congeners are the least reactive, with an estimated atmospheric lifetime of 3 days (Atkinson, 1987). The model includes reaction of the gas phase dioxin species with OH. The rate for this reaction is $3\text{X}10^3$ ppm^{-1}min^{-1}. At present, it does not appear feasible to include the photolysis pathway as realistic decay rates have not been reported.

2.3.4.3.   Polycyclic Organic Matter (POM)

Polycyclic Organic Matter (POM) is not a single compound but rather a whole class of compounds containing two or more fused aromatic rings. In general, POM is semi-volatile and therefore may exist in the gas phase or be associated with particles. REMSAD incorporates the

representation of POM developed for the UAM-TOX model (Ligocki et al., 1992) where three classes of POM are defined based on molecular weight (MW):

NAPH: MW < 160

POM1:   160 < MW < 220

POM2:   220 < MW

NAPH is the most volatile and POM2 the least volatile fraction of POMNAPH is carried in gas phase only in REMSAD. Gas phase species (POM1, POM2) and particulate phase species (POM1P, POM2P) are carried for the other POM compounds.

The gas/particle partitioning algorithm for POM that is used by REMSAD is:

$$f_p = \frac{1}{3.55E7 \times P_L(T)/TSP + 1}$$

where f_p is the particulate fraction, P_L is the subcooled liquid vapor pressure, T is temperature, and TSP is total suspended particulate. TSP estimated in REMSAD from PM_{10}. For POM1 and POM2, PL is calculated as

$$P_L(T) = 1.4X10^{-4}e^{6600(1/298-1/T)},$$

and

$$P_L(T) = 5X10^{-7}e^{7600(1/298-1/T)},$$ respectively, where T is ambient temperature in K.

The reactions of gas phase POM with OH are important and are represented as:

NAPH + OH $\Rightarrow$ 0.02 POM1 + 0.5 NAPH

POM1 + OH $\Rightarrow$ 0.5 POM1 + 0.1 POM2
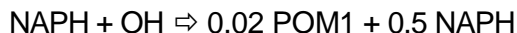
reaction rates for these reactions are $6X10^4 e^{-440(1/298-1/T)}$ and $7X10^4 e^{-440(1/298-1/T)}$ ppm^{-1}min^{-1}, respectively, where T is ambient temperature in K (Atkinson et al., 1987; Atkinson et al., 1990). No reaction of POM2 with OH is included as there are no available data on the reaction rates or products, and the products are likely to be other POM2 species. These simple reactions for POM are solved analytically.

2.3.4.4.   Atrazine (ATRAZ)

Atrazine is a herbicide that inhibits the growth of vegetation. It enters the atmosphere as a gas and subsequently decays by reaction with OH. Atrazine, in gas phase, decays by reaction with OH:

ATRAZ + OH $\Rightarrow$ unknown product,
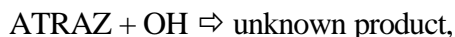
with a reaction rate of $2X10^5$ ppm^{-1}min^{-1}. A gas phase and a particulate phase species are carried for atrazine in REMSAD. The gas/particle partitioning is performed in a manner similar to the POM species above with sub-cooled liquid vapor pressure defined by

$$P_L(T) = 8X10^{-6}e^{7000(1/298-1/T)},$$ where T is ambient temperature in K.

2.3.4.5. *Mercury*

Mercury is volatile in elemental form but involatile in many oxidized inorganic forms and therefore may be present both in the gas and particulate phases. Gaseous mercury species other than elemental Hg may be present in the atmosphere (e.g., organo-mercury compounds). Estimates of mercury emissions include a significant fraction emitted as gaseous, oxidized mercury (EPA,1996).

The chemical transformations of mercury included in REMSAD are based on the review of current status of atmospheric chemistry of mercury presented by Lin and Pehkonen (1999). Prior versions of REMSAD included only the aqueous phase reaction of mercury with ozone. Specific compounds of mercury are not tracked in REMSAD. Species representing the oxidation state of mercury and the phase (gas or particulate) are tracked. The mercury species tracked in REMSAD are HG0 (elemental mercury vapor), HG2 (divalent mercury compounds in gas phase), and HGP (divalent mercury compounds in particulate phase). The reactions in REMSAD cause transfer of mercury mass from one of these states to another. In cloud water, HGP is assumed to dissolve with the solubility of HgO (mercury(II) oxide). In cloud water, some HG2 is assumed to be adsorbed to soot particles (e.g., see Seigneur et al., 1998). The treatment is parameterized via a simple formula. The species PEC (primary elemental carbon) is used as an indicator of the amount of soot present. Fifty-five percent of the dissolved divalent mercury (Hg^{2+}) in aqueous phase is assumed to be adsorbed to soot particles when PEC is 450 ugm/(mole of air) or greater. When PEC is zero, no adsorption takes place. Between these two extremes, the fraction of adsorbed Hg^{2+} is linearly interpolated. REMSAD does not have an internal estimate of chlorine concentrations. Therefore, an input file is required to specify chlorine. The chlorine pathway is considered to be active only at night and chlorine at upper levels is typically set to zero. Chlorine concentrations are supplied at the surface with differing values over the ocean and over land. A typical value used for chlorine over the ocean is 125 ppt (Tokos et al., 1998). Chlorine over land areas is much lower. Discussions with experts suggested a value of 5 ppt over land. Chlorine concentrations are reduced linearly from the surface to zero at a height of 2000 m over the ocean or at a height of 1000 m over land. In order to treat reduction of HG2 by sulfur compounds, the average amount of dissolved SO_2 is estimated during the calculation of the aqueous formation of sulfate (via reaction of SO_2 with H_2O_2, O_3, and O_2). Equilibrium concentrations of $HgSO_3$ and $Hg(SO_3)_2^{2-}$ are calculated and then the production rate of HG0 from $HgSO_3$ is calculated. The pH of cloud water is needed in order to calculate the Henry's law coefficients of some species. In these cases, pH is assumed to be 4.5. Some of the individual species-specific reactions such as photoreduction (for halo-compounds of divalent Hg) and reactions of dimethylmercury by OH, O3, NO3, Cl, O(3 P) have been neglected.

The routine that calculates chemical transformations of mercury is provided with total concentrations of HG0, HG2, and HGP. The routine calculates the fraction in gas and aqueous phases of each of these categories. Gas and aqueous chemical transformations are calculated independently. The routine then recombines the gas and aqueous fractions to return the new total concentrations of HG0, HG2, and HGP.

The following reactions are included in the REMSAD mechanism for mercury:

Reaction	Rate (unit)
For HG0	
Gas phase	
HG0+ $O_3 \rightarrow$ HGP	3.0e-20 (cm^3molecule^{-1}s^{-1})
HG0 + $NO_3 \rightarrow$ HGP	4.0e-15 (cm^3molecule^{-1}s^{-1})(currently disabled)
HG0 + $H_2O_2 \rightarrow$ HG2	8.5e-19 (cm^3molecule^{-1}s^{-1})
Aqueous phase	
HG0 + $O_3 \rightarrow$ HG2	4.7e+7 (M^{-1}s^{-1})
HG0 + OH $\rightarrow$ HG2	2.0e+9 (M^{-1}s^{-1})
HG0 + $Cl_{aq} \rightarrow$ HG2	(See eq. 8 in Lin and Pehkonen, 1999)
HgSO3 $\rightarrow$ HG0	$T\ e^{(31.971\ T - 12595)/T}$ s^{-1} (Van Loon et al., 2000)
For HG2	
Aqueous phase	
HG2 + $HO_2 \rightarrow$ HG0	1.7e+4 (M^{-1}s^{-1})
HG2 + $SO_3^{2-} \leftrightarrow HgSO_3$	5.e+12 (M^{-1})
$HgSO_3 + SO_3^{2-} \leftrightarrow Hg(SO_3)_2^{2-}$	2.5e+11 (M^{-1})
Hg2 + $OH^- \leftrightarrow Hg(OH)^+$	4.27e+10 (M^{-1})
Hg2 + 2 $OH^- \leftrightarrow Hg(OH)_2$	1.74e+22 (M^{-1})
Hg2 + OH^- + $Cl^- \leftrightarrow$ HgOHCl	1.78e+18 (M^{-2})
Hg2 + $Cl^- \leftrightarrow HgCl^+$	2.0e+7 (M^{-1})
Hg2 + 2 $Cl^- \leftrightarrow HgCl_2$	1.e+14 (M^{-2})
Hg2 + 3 $Cl^- \leftrightarrow HgCl_3^-$	1.e+15 (M^{-3})
Hg2 + 4 $Cl^- \leftrightarrow HgCl_4^{2-}$	3.98e+15 (M^{-4})

Source: Lin and Pehkonen, 1999

2.3.5. Transport Processes

Pollutants are transported primarily by advection, that is, by the mean or bulk motion of the air. Accurate representation of the magnitude and variability of the winds within the space-time simulation domain therefore is of key importance in successful application of the REMSAD model.

Diffusion processes also influence the redistribution (or mixing) of pollutants within the modeling domain. Diffusion is driven by turbulent eddies that develop in the atmosphere due to gradients in the atmospheric properties. The effects of diffusion are represented in the REMSAD model using numerical approximations (horizontal diffusion) and using coefficients derived from the meteorological fields (vertical diffusion).

REMSAD is typically applied for the continental scale and for a modeling domain that includes the atmospheric boundary layer, the lower troposphere, and a portion of the upper (or "free") troposphere. The horizontal and vertical extent of the domain and the need to include the upper troposphere derives from the relatively long atmospheric lifetime of particulates and some airborne toxics. Long-range transport can occur in the lower troposphere and even more efficiently in upper troposphere (due to higher wind speeds and more organized airflows) if material is transported into the upper troposphere through convective activity.

2.3.5.1.   Horizontal Advection and Diffusion

The positive-definite advection scheme developed by Smolarkiewicz (1983) is used to represent horizontal advection in the REMSAD model. The Smolarkiewicz advection scheme is a finite-difference scheme that calculates the transport between model cells explicitly. In order to counteract the effects of numerical diffusion, the scheme calculates an anti-diffusion velocity. Successive passes through the transport step using this anti-diffusion velocity minimize the numerical diffusion.

Other descriptions of the Smolarkiewicz scheme are provided by Chock (1991) and Odman (1998).

In REMSAD, the Smolarkiewicz scheme has been adapted to both the cell-centered grid and the staggered grid options. For the staggered-grid configuration (also known as an Arakawa-C configuration), the wind velocities are defined on the grid cell interfaces, reducing the distance used in calculating derivatives of horizontal wind components from $2\Delta x$ to Δx. In certain situations (e.g., a lake breeze convergence zone) this may improve the ability of the REMSAD model to represent vertical transport.

In idealized tests, several other advection algorithms, such as the piecewise parabolic method (PPM) and the Bott scheme, exhibit less numerical diffusion than the Smolarkiewicz algorithm but require significantly greater computation time. These and several other schemes are described by Byun et al. (1999). However, given that there is very little that is known about the properties of horizontal diffusion, it is difficult at present to truly evaluate whether one advection scheme is more appropriate than another for use in current air quality models such as REMSAD. It is possible that numerical diffusion compensates for uncertainties (or underestimates) in the calculated or otherwise specified estimates of horizontal diffusion in air quality models. Consequently, it remains to be seen whether, under representative real-world flow conditions, these other algorithms produce noticeably different and improved solutions from those of the Smolarkiewicz algorithm.

Horizontal diffusion is assumed to be proportional to the horizontal concentration gradient. The proportionality factors (K_X, K_Y) are calculated within REMSAD based on the deformation characteristics of the horizontal wind, following Smagorinsky (1963). The values of Kx and Ky are equal to $0.25/\sqrt{2} *(\Delta x*\Delta y) * D$ where D is the deformation of the wind field. Horizontal diffusion along the lateral boundaries of the REMSAD modeling domain is set equal to zero; this represents a zero-flux boundary conditions for horizontal diffusion.

2.3.5.2.   Optimization of time step selection

The Smolarkiewicz algorithm is implemented as a one-dimensional advection scheme in REMSAD. Therefore, horizontal transport in calculated in the x (E-W) direction along each row of the domain for all layers and then in the y (N-S) direction along each column of the domain for all layers. The one-dimensional nature of the algorithm along with the time step structure

described earlier in this section allows an efficient solution method to be implemented for the horizontal advection. Typically, the time step for the advection step in the model would be selected based on numerical stability given the maximum wind speed and the grid spacing. The driving time step selected in this manner is usually constrained due to the high wind velocities found in the upper layers of the model domain. Thus, the model is restricted to an advective time step, which, throughout most of the modeling domain, is unnecessarily small. In order to overcome this restriction, the model code has been restructured in order to reduce the overall computational time required for a REMSAD modeling application.

Since the main limitation on the size of the time step in REMSAD is the selection of the advective time step based on the maximum wind speed and the minimum grid spacing in the entire modeling domain, a means of relaxing this restriction was investigated. First, it was recognized that within the framework of the time-splitting approach to the solution of the species continuity equation, each of the various processes being simulated could be solved using a time step most appropriate to the particular process. In other words, if we consider, for example, the vertical advection/diffusion and the horizontal advection/diffusion processes we see that based on numerical stability criteria the vertical advection process can be solved using a much larger time step than is required for the horizontal advection. A similar situation exists among the various other processes, including injection of emissions, removal processes (deposition) and chemical transformations. A technique was therefore implemented to incorporate this "time-step nesting" procedure. In order to accomplish this, the code was restructured such that the overall time-splitting is done in a symmetrical manner. That is, assuming that the chemistry calculations are performed on the smallest time scale followed by horizontal advection/diffusion and then vertical advection/diffusion, the code was structured such that a half time step is taken for vertical advection/diffusion, a half time step is taken for horizontal advection/diffusion and finally a full time step for the chemistry computations. This is then followed by a half time step for the horizontal and vertical transport processes in a reverse order (i.e., horizontal advection/diffusion followed by vertical advection/diffusion) in order to complete a full global time step in the model.

In addition to allowing the various physical processes to run at different time steps, the numerical calculations within a particular process are allowed to proceed at varying time steps in different parts of the grid as well. In particular, the horizontal advection, which typically takes 40-50% of the overall computing time within the model, has been restructured to take advantage of the fact that, throughout most of the computational grid, stability requirements would allow a much larger driving time step than that dictated by the maximum wind speed and minimum grid size within the entire domain. Thus, when simulating the horizontal advection, a variable time step is used on each modeled layer, and within each layer, variable time steps are used for integration of the advection equation along each row and column of the grid. Each process is repeated at the corresponding time step until a time equal to the outer time step has been completed.

In addition to restructuring the code and using variable time steps for each of the major processes, specific algorithms were examined with the ultimate goal of selecting the most accurate and appropriate routines that would require the minimum amount of computing time. To date, only the second-order polynomial Bott's scheme employed for the vertical advection algorithm has been replaced with a simpler upstream differencing algorithm which gives essentially the same results while achieving an approximately 5% decrease in overall runtime.

2.3.5.3. *Vertical Advection*

Vertical advection is driven by the vertical component of the wind field, which is calculated by REMSAD using the conservation of mass equation:

$$\partial w/\partial z = - (\partial u/\partial x + \partial v/\partial y)$$

It is expected that the vertical wind component, *w*, is much smaller than the horizontal wind components. Vertical velocity is typically greatest under convective conditions (e.g. within convective clouds), and terrain- or sea-breeze-induced convergence zones.

2.3.5.4. *Vertical Diffusion*

Diffusion of pollutants in the vertical is assumed to be proportional to the vertical concentration gradient. The proportionality factor is termed the vertical exchange or eddy diffusivity coefficient (K_V).

Vertical exchange coefficients are specified as an input field for REMSAD. As discussed in Section 4 of this user's guide, the gridded K_V values can be obtained directly from the output of a dynamic meteorological model or can be calculated (diagnosed) using other of the meteorological input parameters (e.g., wind speed, stability or turbulent kinetic energy). The K_Vs comprise a three-dimensional array; the values for each grid cell are applicable to the top of each model layer. A zero-flux boundary condition is applied for vertical diffusion at the top of he modeling domain. No K_V value is specified for the lower boundary of the domain; in this case the flux from the lowest layer to the surface is represented in the model by (dry) deposition.

2.3.6. Cloud Dynamics

The presence of clouds affects a number of processes in REMSAD. In the section "Aqueous-Phase Sulfate Chemistry " above, the role of clouds in sulfate formation is discussed. In the section on "Wet Deposition" below, the role of clouds, cloud liquid water, and rainfall on the removal of airborne pollutants is discussed. The effect of cloud cover on photolysis rates in discussed under "Photolysis Rates" above. In this section, the treatment of the effect of clouds on the vertical distribution of pollutants is discussed.

It has been generally recognized that clouds have a major role in the vertical redistribution and removal of pollutants (Chang et al., 1987; Lin et al., 1994). The vertical redistribution of pollutants within clouds can be conceptualized as the net of two processes: (1) upward and downward vertical advection (due to convection and turbulent mixing) and (2) downward vertical transport due to precipitation. Cloud type, convective intensity, precipitation rate, liquid water content, and vertical temperature profile determine the effectiveness of the redistribution processes. The vertical extent of the cloud is also an important parameter in determining the vertical distribution of pollutants.

2.3.6.1. *Estimating Cloud Type, Vertical Extent, and Coverage*

Within REMSAD, clouds are classified as either stratiform or convective. Stratiform clouds are not associated with significant vertical motions or vertical extent, but can produce precipitation. Convective clouds are typically characterized by moderate to strong vertical velocity components; convection can be shallow (a few meters) or deep (up to approximately 1 km). Cloud type (stratiform versus convective) and cloud parameters (top, bottom, freezing level, cloud cover fraction) within REMSAD are estimated following Anthes et al. (1987) and Anthes

(1977). The diagnosis is based on the corresponding vertical profiles of temperature, mixing ratio (water vapor), and pressure.

The base or lowest level of the cloud is estimated by calculating the lifting condensation level (LCL). In REMSAD, this level is estimated to be the level below 700 mb with the highest estimated equivalent potential temperature. Equivalent potential temperature is the temperature that an imaginary air parcel that is lifted from the ground would attain due to adiabatic cooling (according to a dry adiabatic lapse rate of 1°C/km) and condensational heating (assuming a constant mixing ratio). The vertical distribution of equivalent potential temperature is used to determine the presence of convective instability in the modeled atmosphere. Conceptually, if equivalent potential temperature decreases with height, rising parcels will be warmer and more buoyant that the environment and will continue to rise (resulting in convection). The level with the highest equivalent potential temperature is assumed to represent the starting point for convection or the LCL. The model level immediately below the LCL is considered to be the cloud-base level (s_b). The equivalent potential temperature at the cloud base is designate q_{ec}.

The top of the cloud is defined as the level for which the saturation equivalent potential temperature is greater than that for the base of the cloud. The saturation equivalent potential temperature (q_{es}) is reached when all moisture is condensed. Thus when an imaginary parcel reaches this level, no further condensation heating occurs and it is no longer buoyant with respect to its environment. In REMSAD, the first level for which $q_{es} > q_{ec}$ is specified to be the top of the cloud. This level is designated s_t. Note that because of the typical relatively coarse vertical resolution in the upper part of the modeling domain, we have assumed no convective overshooting (in which convection extends beyond the saturation equivalent potential temperature level).

Cloud type is assessed based on the potential for convective activity. To determine if convection is possible within the cloud, four diagnostic tests are performed. First, the available buoyant energy (*ABE*) is calculated. If *ABE* is positive, then convection is possible. *ABE* is determined from:

$$\mathrm{ABE} = \int_{s_t}^{s_b} (q_{ec} - q_{es}(s))\, ds$$

If the ABE is positive, then the strength and depth of the convection is examined using diagnostic formulae (Anthes, 1977). The strength of the convection is estimated using a mixing coefficient.

$$m_d = \frac{-s_{cb}[q_{ec} - \overline{q}_e]}{\int_{s_t}^{s_b} [q_e(s_b) - q_e(s)]\, ds}$$

where s_{cb} is the sigma-based vertical velocity at the cloud base and is assumed to be -1×10^{-3} (sigmas)s^{-1} and q_e is the mean environmental equivalent potential temperature of the whole cloud layer. If the mixing coefficient is positive, then convection is possible.

The depth of the convection is assumed to be equal to the cloud depth. If the cloud depth is greater than 0.3 (sigmas), then convection is possible.

Finally, for convection to be possible sufficient moisture convergence must be available within the whole grid. The moisture convergence within the grid column, M_t, is determined from:

$$M_t = -\frac{1}{g}\int_0^1 \nabla \cdot (p^*Vq_v)\,d\mathbf{s} > M_c$$

where g represents acceleration due to gravity, V is the horizontal wind speed vector, and q_v is the mixing ratio of water vapor, and $p^* = p_s - p_t$ with p_s and p_t being the pressure at the surface and the top of model domain, respectively. If M_t is diagnosed as being greater than the critical moisture convergence threshold, M_c, chosen as 3×10^{-8} kg m^{-2} s^{-1} (per Lin et al., 1994), then convection is occurring.

If all four of these tests are met, the REMSAD cloud type is convective. Otherwise the cloud is considered to be stratiform.

If convection occurs, then according to Anthes (1977) the convective cloud cover fraction can be expressed for each grid cell by

$$c_d = \frac{(1-b)\,gM_t}{4.3\times10^{-3}}$$

where (1 - b) is the fraction of the grid column assumed to condense and precipitate, b is assumed to moisten the grid column and is a function of the mean relative humidity RH of the column

$$b = 2(1-\overline{RH}), \quad \overline{RH} \geq 05,$$
$$b = 1.0, \quad \quad \overline{RH} < 0.5.$$

The value 4.3×10^{-3} cb s^{-1} (centibars per second) is based on a typical value for a deep convective cloud.

If stratiform clouds are diagnosed, then the cloud cover is calculated according to the parameterization suggested by Geleyn (1981),

$$c_s = \left(\frac{RH - RH_c}{100 - RH_c}\right)^2, \quad RH \geq RH_c$$

in which the threshold relative humidity (percent), RH_c, is calculated by

$$RH_c = 100 - 100c_1\frac{p}{p_s}\left(1-\frac{p}{p_s}\right)\left[1 + c_2\left(\frac{p}{p_s} - 05\right)\right]$$

in which $c_1 = 2$ and $c_2 = \sqrt{3}$.

Additional constraints are also placed on the stratiform cloud before allowing the calculation of the vertical redistribution of pollutant mass. These constraints are:

- Maximum cloud coverage in the grid cell is at least 10 percent.

- The depth of the cloud layer is greater than 0.1 in sigma units (roughly 1000 m in lower layers).

- The bottom of the cloud layer is no higher than 3000 m above ground level (agl).

2.3.6.2.   Net Vertical Distribution for Deep Convective Clouds

The nonlocal convective PBL scheme of Blackadar (1979) is the basis for calculating the tendency for mixing within deep convective cumulus clouds. Above the lowest model layer, the tendency (or change in concentration with time) for a trace species α in layer *k* within the cloud is assumed to be proportional to (1) cloud cover and (2) the difference in concentration (or mixing ratio) for the species for that layer (α_k) and for all layers (averaged) below the cloud (α_{sc}),

$$\left(\frac{\partial a_k}{\partial t} \right)_d = m_d\, c_d\, (\overline{a}_{sc} - a_k)$$

where $\overline{a}_{sc}$ is expressed as

$$\overline{a}_{sc} = \frac{\int_{s_b}^{1} a(s)\,ds}{1 - s_b}$$

Applying mass conservation, the tendency due to deep convective mixing within the cloud should balance with those in the sub-cloud portion of the modeling domain. This is expressed mathematically as:

$$\sum_{k(s_b)}^{k(s_t)} \left[\left(\frac{\partial a_k}{\partial t} \right)_d \Delta s_k \right] = - \sum_{k(1)}^{k(s_b)+1} \left[\left(\frac{\partial a_k}{\partial t} \right)_d \Delta s_k \right]$$

Lin and coworkers (1994) further assume that the tendency in each sub-cloud layer is proportional to the mixing ratio of the species in the layer if the tendency in the cloud layer is negative (i.e., there is a net flux out of the cloud). Conversely, if the tendency in the cloud layer is positive (i.e., there is a net flux into the cloud), then the tendency in each sub-cloud layer is inversely proportional to the mixing ratio. In REMSAD, the tendencies are calculated for each layer and species. The calculated tendencies are used to adjust the concentrations for each of the REMSAD species. This yields a new vertical distribution.

2.3.6.3.   Net Vertical Distribution for Stratiform Clouds

The parameterization scheme for stratiform clouds is taken from Lin et al. (1994) in which vertical mixing within cloud layers is treated using explicit K-theory. A typical turbulent mixing coefficient (K_v) in stratiform clouds is of the order 50 $m^2\ s^{-1}$. This nominal K_v value provides the basis for the redistribution calculation. It is adjusted to be specific to each cloud layer based on the amount of moisture present in the cloud layer. The adjusted turbulent mixing coefficient, K_p, is then used to adjust or redistribute the species concentration according to:

$$\alpha_k = \alpha_k + K_p\,(\alpha_{k+1} - \alpha_k) - K_{p-1}\,(\alpha_{k+1} - \alpha_k)$$

where α_k is the adjusted mixing ratio or concentration of species α in the *k*th layer. This implicitly limits the exchange (or redistribution) to two neighboring layers.

2.4. Wet Deposition

Wet deposition is the scavenging of gasses and particulates from the atmosphere by precipitation, and their subsequent deposition (in rainwater) to the surface. Wet deposition is one of the mechanisms for the removal of pollutants from the REMSAD atmosphere. Separate treatments are used for gasses and particulates.

2.4.1. Gaseous Wet Deposition

The gaseous wet scavenging algorithm in REMSAD is based on Henry's law and specifically Hales and Sutter (1973). According to Henry's Law, the dissolved concentration of a gas in water is proportional to the partial pressure of the gas over the water. Mathematically, this can be expressed as $[A(aq)] = H_A P_A$, where $[A(aq)]$ is the aqueous concentration of the gas in mole/liter, H_A is the Henry's Law constant for the gas, and P_A is the partial pressure of the gas in atmospheres. Some gases, such as SO2, react with the hydrogen ions present in water and are effectively more soluble than predicted by the above law. The increased solubility is accounted for by using the effective Henry's law coefficient, which is dependent on the hydrogen ion concentration. Expressions for the effective Henry's law coefficients are included in REMSAD for the standard simulated species. The approach developed by Hales and Sutter involves calculating the amount of gas dissolved in water and the rate at which the liquid water rains out of the system. It originally focused on sulfur dioxide. As used in REMSAD, it has been generalized for any gaseous species (assuming low concentration).

The REMSAD wet deposition algorithm considers six gaseous (NO, NO_2, SO_2, NH_3, VOC, HNO_3) plus seven toxic species. Temperature dependencies for Henry's Law constants are incorporated for all species. Solubility (K_H), ionization (K_{1D}, K_{2D}), and vapor pressure constants for the toxic species were obtained from recent literature.

The following scavenging rate was derived by Hales and Sutter (for derivation, see below).

$$RWET = RANM / H(LWC + SOL),$$

where SOL is solubility, LWC is liquid water content, H is the layer depth, and RANM is rainfall in m/hr. This scavenging rate is used to adjust (reduce) the species concentration in each model layer. Scavenging is applied successively to each layer and the total flux (wet deposition to the surface) is the sum of the mass removed from all layers that extend from near cloud top to the ground.

According to Hales and Sutter, the ratio of the gaseous concentration of a given species to the liquid-phase concentration (C_g / C_l) in the atmosphere can be expressed as:

$$SOL = C_g / C_\ell = 1 / \left(K_H + \frac{K_{1D} K_H}{[H^+]} + \frac{K_{2D} K_{1D} K_H}{[H^+]^2} \right)$$

where

C_l	=	liquid-phase concentration (mol/l water)
C_g	=	gaseous-phase concentration (atm)
$[H^+]$	=	concentration of hydrogen ions (mol/l water)
K_H	=	species-dependent Henry's Law equilibrium constant

and K_{1D} and K_{2D} are species-dependent first and second ionization constants. For the purpose of estimating the hydrogen ion concentration, REMSAD assumed a cloud water pH of 4.5.

Conservation of mass requires the following relationship between gas-phase concentration, liquid-phase concentration, and total (liquid and gas) concentration (C_o):

$$C_g + (C_l \times \text{LWC}) = C_o$$

where *LWC* is the liquid water content (of the atmosphere). Substituting from above and rearranging terms we can express the liquid-phase concentration as:

$$C_l = C_o/(\text{LWC} + \text{SOL})$$

where *LWC* is taken from the rain liquid water input data file. The scavenging of pollutant mass by precipitation can be generally expressed by the equation:

$$W_i = \rho_w \bullet \text{RANM} \bullet \chi_i/H$$

where

W_i	=	mass of species *i* material scavenged per unit volume of air per unit time
ρ_w	=	the water density
χ_i	=	mass of species i scavenged per unit mass of water
H	=	the layer depth.

The scavenging rate for gaseous removal, RWET, can be expressed by dividing the above equation for W_i by the species concentration, C_o:

$$RWET = W_i \, / \, C_o = \left(r_w \bullet RANM \bullet c_i \right) / HC_o$$

By substituting into the above expression and using the alternative definition for $C_l = \rho_w \cdot \chi_i$.

$$RWET = RANM \, / \, H(LWC + SOL)$$

2.4.2.   Particulate Wet Deposition

Wet deposition of aerosols in REMSAD utilizes many of the relationships established by Scott (1978), which relate rainfall rate and cloud type to fraction of ambient sulfate within rainwater reaching the ground. The equations have been expanded from sulfate only to treat any aerosol species. Non-sulfate aerosols are assumed to scavenge at a constant fraction of the sulfate rate. This fraction can be specified by the user in the CHEMPARAM file for each species and is dependent upon on each species' hygroscopic nature and its affinity to exist with other hygroscopic species. Settings for this fraction in current CHEMPARAM files is as follows:

PNO3	1.0
GSO4	1.0
ASO4	1.0
NH4N	1.0
NH4S	1.0
SOA	0.5
POA	0.2
PEC	0.2
PMFINE	0.2
PMCOARS	0.2

For aerosols smaller than 1μm in diameter, it is assumed that the capture of aerosols by phoretic attachment or Brownian motion is negligible and that the principal scavenging mechanism is the nucleation of cloud droplets around aerosols followed by particle growth through coalescence and accretion of cloud droplets to sizes large enough to fall through the cloud as precipitation. Aerosols larger than 1μm are removed strictly by impaction with falling raindrops.

For the portion of clouds in which Bergeron (mixed cloud of ice crystals and liquid water) processes for rain initiation occurs, it is expected that aerosols do not participate in the nucleation of cloud ice crystals, and therefore are not present in ice crystals as they coalesce into larger precipitating crystals. In warm clouds, including both stratiform and convective clouds, nucleation and coalescence are assumed to be the dominant process for cloud droplet growth with aerosols acting as nuclei. However, the cloud layer depth over which these processes occur is treated separately for stratiform and convective clouds.

Relationships between rainfall rate, median drop size and fallspeed, and precipitable water content have been developed by Scott (1978) and Kessler (1969) as:

$$V = 130D^{0.5}$$

$$D = 8.95 \times 10^{-4} R^{0.21}$$

$$M = 0.071R^{0.88}$$

where V is fallspeed or velocity (m s^{-1}), D is median drop diameter (m), M is precipitable water content (g m^{-3}), and R is the rainfall rate converted to mm h^{-1}.

These relationships are used in REMSAD to determine the precipitable water content, drop diameter, and velocity of the hydrometeor at cloud base and at top of the riming zone. The depth over which active hydrometeor growth is occurring is estimated based on the particular layer structure of the cloud and rainfall rate within the cell. A typical residence time t in the riming zone of 384 s for stratiform clouds and 769 s for convective clouds has been used to initially estimate the depth of the riming zone . Final residence time is determined once the top of the riming zone has been determined. The residence time is then used to calculate the vertically averaged cloudwater mass, $\overline{m}$ whose relationship is expressed as:

$$\overline{m} = (1/C_1 t)(3.12 + 0.88 \ln R)$$

where $C_1 = 5.2 \times 10^{-3}$ m^3 g^{-1}s^{-1} (for raindrops) and t is time. The washout rate w_{rat} for the layer just above the riming zone is given by:

$$w_{rat} = M_o/\overline{m} - t$$

where $-t = 435R^{-0.71} + 1200$ based on continental warm phase-clouds and

$$M_o = 3.15 \times 10^{-3} \text{ g m}^{-3}.$$

If the cloud type is stratiform and the layer just above the riming zone is freezing, then the washout rate is considered negligible and the contribution from this layer is ignored.

To determine the washout rate for each cloud layer within the riming zone the precipitable water content M_k is determined for each layer from the expression:

$$M_{k+1} = M_k / \exp(-C_1 \overline{m} \, t_k)$$

where

M_{k+1} =   precipitable water within layer $k + 1$,

M_k =   precipitable water within layer k,

t_k =   time hydrometeor is within layer k.

The w_{rat} for each layer k is calculated in an analogous manner to the top layer,

$$w_{rat} = M_k / \overline{m} \, t_k$$

For the layer just below the cloud base down to layer one the w_{rat} removes particles strictly through impaction with falling raindrops. The expression for their removal is given by:

$$w_{rat} = 2.14 \times 10^{-2} \, C_1 R^{0.88}$$

with an assumed inertial impaction efficiency of 0.3.

The effective washout rate fraction for each species is then adjusted logarithmically for the hygroscopic affinity (fc) and aerosol size distribution of each species and the aerosol available for incorporation into the cloud water. This washout or scavenging rate is used to adjust (reduce) the aerosol concentration in each model layer. Washout is applied successively to each layer and the total flux (wet deposition to the surface) is the sum of the mass removed from all layers that extend from near cloud top to the ground.

2.5. Dry Deposition

The dry deposition algorithm in REMSAD is based on the scheme in the Regional Acid Deposition Model (RADM) as described by Wesely (1989). A more complete description of this algorithm is provided by Scire (1991). In this methodology, the flux of pollutant material to the surface (the lower boundary of the modeling domain), F_0, is expressed as a product of the concentration in the lowest model layer (C_i) and the deposition velocity (V_d):

$$F_0 \quad = \quad -C_i \; V_d$$

Thus dry deposition of a given species is directly proportional to the concentration of that species within the lowest model layer.

The deposition velocity is estimated as an inverse sum of a series of resistances (such that the greater the resistance, the lower the deposition velocity). For gaseous species this is expressed as follows:

$$V_d \quad = \quad \frac{1}{R_a + R_b + R_s}$$

where R_a is aerodynamic resistance, R_b is boundary-layer resistance, and R_s is surface resistance. These represent the effects of turbulent diffusion (within the lowest layer), molecular diffusion (that occurs very near the surface), and finally uptake at the surface (once the surface is reached).

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The aerodynamic resistance (R_a) is dependent on the surface characteristics and atmospheric stability conditions. It is calculated from two surface-layer similarity parameters: the friction velocity and the Monin-Obukhov length (see Gray et al., 1991).

The boundary or quasi-laminar layer resistance (R_b) represents the process of molecular diffusion of the transport of pollutants through the laminar layer around solid objects and is highly dependent on the Schmidt number (the ratio of air kinematic viscosity to the molecular diffusivity of the pollutant in air; see Gray et al., 1991). Note that molecular diffusion is inversely proportional to the molecular weight.

The surface resistance (R_s) is actually a set of parallel resistances associated with (1) leaf stomata, (2) leaf cuticles, (3) lower canopy resistances (e.g., bark, stems, etc.), and (4) surface soil, litter, and water (see Wesely, 1989). Surface resistance (resistance to uptake) is both species and surface dependent.

The deposition velocity of particulate species also depends on particle size distribution and density. Particles have a sedimentation velocity (V_{sed}) or fall-out rate that can be a significant component of the deposition velocity for large particles. Very small particles have a negligible sedimentation velocity and behave in a manner similar to gases. In REMSAD particle deposition velocity is calculated as:

$$V_d \;=\; V_{sed} \;+\; \frac{1}{R_a + R_b + R_a R_b V_{sed}}$$

where V_{sed} (m/s) is given by the equation

$V_{sed} = g\, d_p^{\,2}\, (? - ?_{air})\, C/18\mu,$

where $?$ is the particle density (g/m3), $?_{air}$ is the air density, g is the acceleration due to gravity (9.8 m/s2), dp is particle diameter (m), and μ is the viscosity of air. C is the slip correction factor given by

$C = 1 + 2(l/d_p)[A_1 + A_2 exp(-A_3 d_p/l)]$, where l is the mean free path, and A_1, A_2, and A_3 are 1.257, 0.4, and 0.55 (Friedlander, 1977).

2.5.1.   Calculation of Micrometeorological Parameters

Two meteorological scaling parameters (with a basis in similarity theory) are needed for the calculation of the aerodynamic resistance term used in by the dry deposition algorithm. These are the friction velocity and the Monin-Obukhov length and are calculated within REMSAD from the gridded wind, temperature, and pressure input fields. These scaling parameters for velocity and length are essentially invariant with the atmospheric surface layer and enable the calculation of various turbulence-related effects. The approach to calculation of these parameters is based on similarity theory. Temperature and pressure for the surface and the lowest model layer are used to calculate a potential temperature gradient, which is then combined with wind speed for the lowest model layer to determine stability within the layer. Friction velocity and Monin-Obukov length are then calculated following the formulation of Louis (1979) for each land-use category. These parameters vary according to land-use category due to differences in roughness length, which is also considered in the calculation. Wind speed at a height of 10 m agl is also estimated.

Recognizing that the roughness of a water surface depends on surface stress (i.e., wind speed) water roughness length is specifically calculated from friction velocity and subsequently used in the calculation of the resistance terms for grid cells containing water surfaces.

2.5.2.   Calculation of Resistance Terms

The surface (10 m) wind speed, friction velocity, and Monin-Obukhov length for each land-use category within a grid cell are used to calculate aerodynamic and boundary resistances for each land-use type in that cell. The resistances are combined with the land-use-dependent surface resistance to obtain a land-use-dependent deposition velocity. The velocities are then weighted by fractional area covered by each land-use type within the grid cell to obtain a single deposition velocity for each grid cell for each species. Other key effects that are incorporated into the calculation of the resistance terms include moisture stress, differences due to water surfaces, and surface moisture.

2.5.2.1.   Effects of Moisture Stress on Stomatal Resistance

Stomatal resistance, which controls daytime gaseous dry deposition to vegetated surfaces via the surface resistance term, increases markedly during periods of moisture stress (Scire, 1991). The deposition algorithm in REMSAD identifies three vegetation states for each grid cell: active unirrigated vegetation in unstressed conditions or irrigated vegetation (State A), active unirrigated vegetation in stressed conditions (State B); and inactive vegetation (State C). Of these states, however, State A is used almost exclusively since data indicating one of the other two states is usually not available. The resistance is approximated for each state as follows:

- For State A, stomatal resistance is parameterized in terms of a reference resistance (which is season and land-use dependent), solar radiation, and surface air temperature. Solar flux is calculated as a function of solar zenith angle, and adjusted directly by the percentage of cloud cover for each cell. A surface air temperature correction factor to stomatal resistance is also included. Default values for minimum, maximum and optimum temperatures for stomatal closing of 0, 40, and 20°C, respectively, are used.

- For State B, which by definition corresponds to minimum stomatal opening, stomatal resistance is arbitrarily set to a multiple of the resistance for State A. The multiplication factor is equal to 10.

- For State C, stomatal resistance is set to a large value (1.0×10^5) that effectively prevents deposition.

For applications in which a lack of data does not allow either accurate determination of moisture stress conditions or the breakdown of irrigated versus unirrigated vegetation (most cases), only state A is considered.

2.5.2.2.   Deposition to Water Surfaces

To accommodate that the deposition to water surfaces can be rapid for many soluble gases a formulation for surface resistance over water based on the work of Slinn et al. (1978) is used by REMSAD. In liquid-phase, resistance is given by

$$R_s = \frac{H}{a_* \ k_l} \tag{2}$$

where H is the Henry's law coefficient, a_* is an effective enhancement of solubility of each gas in water, and k_l is the liquid-phase transfer velocity, which includes the effects of surface stress. Slinn et al. (1978) expressed k_l in terms of surface friction velocity u_* over water as:

$$k_l = 4.8 \times 10^{-4} \ u_*$$

2.5.2.3.   *Effects of Surface Moisture*

The REMSAD dry deposition algorithm includes modifications to the surface resistances for dew- and rain-wetted surfaces per Wesely (1989). The extent of dew is estimated internally by the REMSAD based on relative humidity and wind speed. As suggested by Scire (1991), a formula given by Wesley and Lesht (1988) is used to determine that dew is present when:

(100 – RH) (u + 0.6) < 19, where RH is the relative humidity (%) and u is the wind speed (m/s). As recommended by Wesley, dew wetted surfaces have enhanced deposition for SO2 and other soluble species but increased resistance for ozone. For rain wetted surfaces, resistance to uptake is increased for all species.

2.6. Treatment of Plume Rise

Plume rise in the REMSAD is based on the treatment developed for the Gaussian dispersion model TUPOS (Turner et al., 1986). Plume rise is calculated based on stack parameters and several of the gridded meteorological inputs. These are used to determine the stability characteristics within each layer of the model as well as to calculate explicit buoyancy and momentum flux terms. The method calculates plume rise using both buoyancy and momentum based approaches and then uses the larger values from the two approaches to represent plume rise. If plume rise exceeds the top of the layer containing the stack top, it is recalculated based on the local stability of the next higher layer In this case residual buoyancy flux into that layer is also considered (momentum flux applies in the stack layer only). Once final plume rise is established (i.e., when the calculated rise does not exceed the top of the layer for which the calculations are made), the results are modified to accommodate stack-tip downwash if wind speeds are sufficiently higher than the exit velocity. The details of the plume-rise algorithm are provided below.

2.6.1.   Neutral or Unstable Atmospheric Conditions

For neutral or unstable conditions, the momentum-based plume rise (ΔH_{um}) is determined from

$$\Delta H_{um} = \frac{3 \ d \ v_s}{u}$$

where d is the stack diameter (m), v_s is the stack exit velocity (m/s), and u is the wind speed (m/s).

For these same conditions, buoyant plume rise (ΔH_{ub}) is taken as the lesser of

$$\Delta H_{ub} = 30(f/u)^{3/5} + z_b$$

and

$$\Delta H_{ub} = 24(f/u^3)^{3/5}\left[h_s + 200(f/u^3)\right]^{2/5} + z_b$$

where h_s is physical stack height (m), f is buoyancy flux, and z_b is the vertical distance between the stack tip and the height of the layer in which plume rise is calculated.

Buoyancy flux f is calculated from stack parameters for the layer containing the stack, but is set to residual flux f_r entering the bottom of any higher layer. If the buoyant plume rise exceeds the top of the layer under consideration, the residual flux into the next higher layer is calculated as follows (depending on which buoyancy equation was used):

$$f_r = u\left(\frac{\Delta H_{ub} - z_t}{30}\right)^{5/3} \text{ or}$$

$$f_r = 0.0055(\Delta H_{ub} - z_t)\,u^3\left(1 + \frac{h_s}{\Delta H_{ub} - z_t}\right)^{-2/3}$$

where z_t is the height of the top of the layer containing the plume relative to stack tip.

The plume rise for neutral or unstable conditions is taken as the larger of the momentum-based and buoyant plume rise values.

2.6.2. Stable Atmospheric Conditions

Under stable conditions, momentum-based plume rise is taken as the lesser of ΔH_{um} (momentum-based plume rise for neutral or unstable conditions) and ΔH_{sm}:

$$\Delta H_{sm} = 0.646\left(\frac{v_s^2\,d^2}{T_s\,u}\right)^{1/3} T^{1/2}\left(\frac{\partial q}{\partial z}\right)^{-1/6}$$

where T is the temperature for the model layer, T_s is the stack temperature, q is the grid-based potential temperature, and the remainder of the variables are defined above.

Under stable conditions a uniform "top hat" plume distribution is assumed, with the bottom of the plume one-third as high as the plume top (and plume center two-thirds as high) relative to the stack tip. Stable buoyancy rise of the top of the plume ΔH_t is taken as the lesser of

$$\Delta H_t = \left(\frac{1.8\,f\,T}{u\,\frac{\partial q}{\partial z}} + z_b^3\right)^{1/3} \text{ and}$$

$$\Delta H_t \;=\; \left(\frac{4.1\,f\,T}{f_0^{\,1/3}\dfrac{\partial \boldsymbol{q}}{\partial z}} \;+\; z_b^{8/3} \right)^{3/8}$$

where f_0 is stack tip buoyancy flux and f can be either f_0 or f_r, depending point of calculation.

For stable conditions, plume rise is taken as the larger of stable momentum rise and buoyancy rise of the plume top. If buoyancy rise is selected and the calculated plume top is above the top of the layer in which the plume is located, residual flux is calculated from equation 3 (if buoyancy equation 1 was used) or equation 4 (if buoyancy equation 2 was used):

$$f_r \;=\; f \;-\; 0.56\,\frac{\partial \boldsymbol{q}}{\partial z}\,\frac{u}{T}\left(z_t^3 \;-\; z_b^3\right)$$

$$f_r \;=\; f \;-\; 0.24\,\frac{\partial \boldsymbol{q}}{\partial z}\,\frac{f_0^{\,1/3}}{T}\left(z_t^{8/3} \;-\; z_b^{8/3}\right)$$

where f is either f_r from the previous layer or f_0 in the layer containing the stack.

2.6.3. Final Determination of Plume Rise

The calculation of plume rise continues layer-by-layer using the appropriate equations for stable or neutral-unstable conditions until the plume rise height remains within a given layer. This is then taken as the final plume rise.

2.7. Tagging Scheme for Mercury and Cadmium

Sensitivity simulations involving reduction of emissions, elimination of a particular emissions category or elimination of a particular emissions source are often used to assess the effect of emissions sources on ambient concentrations. In addition, some species, in particular mercury, have global background concentrations that are significant compared to their known emissions. It is therefore often desirable to be able to estimate in a simulation the contribution of the background concentration to the simulated concentration of the species. In order to facilitate this type of sensitivity simulation, a "tagging" scheme for cadmium and mercury has been implemented in REMSAD.

It should be noted at the outset that the information provided by exercising the tagging scheme can also be gained by conducting separate sensitivity simulations. The tagging scheme has some advantages over this method in that some computer time is saved by not having to repeat some common operations (such as the input/output associated with data files, calculation of certain meteorological properties, etc.) and that the results of the tagged species (essentially the results of several sensitivity simulations) are contained in the same output files, which can facilitate analysis. The use of the tagging scheme also encourages careful planning of the simulation, which can lead to more useful simulation results.

The implementation of the tagging scheme in the model code is relatively straightforward. For mercury, three species named HG0-1, HG2-1, and HGP-1 are built into the model, which have the properties of elemental mercury, gas phase divalent mercury and particulate mercury. (See

the discussion of the mercury chemistry elsewhere in this document.) In addition to these species, other species named HG0-n, HG2-n, and HGP-n are included where n is an integer. These species also have the properties of elemental, divalent gas, and particulate mercury. That is, HG0-n reacts in the same way with ozone as does HG0-1; HG0-n deposits in the same way as HG0-1; HG0-n has the same molecular weight as HG0-1; and so forth. A similar set of species is available for cadmium as CD-1, CD-2, etc. Cadmium is treated as a particulate species that does not have a variety of chemical states so there is only one species per tag instead of three per tag as in the case of mercury. Currently the model is configured for up to 24 mercury tags or 10 cadmium tags.

The recommended procedure for setting up a tagging simulation is to prepare emissions from all mercury emissions sources for the –1 tag. Boundary conditions for the –1 tag should be set to typical background concentrations. The simulation results for the –1 tag species will therefore be a "standard" simulation of mercury (or cadmium). The simulated concentrations for the –1 tag would be the simulated ambient mercury concentrations and can be compared to observed data for model validation purposes.

Other species can be set up to tag specific sources of mercury. A tag can be set up to track the background concentrations by setting the –2 tag to the same background concentrations as the –1 tag species. For the background tag, the emissions of the –2 species should all be zero. An emissions tag for mobile sources can be set up by making the emissions of the –3 tag equal to the mobile emissions of the –1 tag species. The background concentrations of the –3 tag species should be zero so that only the mobile source emissions contribute to the –3 tag species concentrations.

Other emissions categories can be tagged similarly. In setting up the tagged emissions categories, they should be split such that the separate categories add up to the emissions of the –1 tag. In this way, the sum of the concentrations of the separate tags (-2 through –n) can be compared to the –1 tag to get an estimate of the discrepancy that may be present in the tagged species compared to using one overall species. It is also possible to estimate the effect of a reduction in a source category on ambient concentrations by scaling the tag concentrations associated with that category. The effect of changes in background concentration can be estimated by scaling that concentrations of the –2 tag. For instance if all background concentrations are reduced by a factor of 2, then the simulated concentration of the –2 tag could be adjusted by a factor of 2, added to all the emissions tag species and that would be the estimate of the new ambient concentrations.

Many other analyses are possible including calculation of percent contribution to deposition or concentrations, summing of tags to estimate contribution of groups of sources and so forth.

3. REMSAD APPLICATION

In this section of the user's guide, we briefly outline and provide guidelines for the application of the REMSAD modeling system. This information is intended to assist and provide some examples and perspective to new or first-time users of the modeling system.

Once it has been decided that REMSAD is the right model for your application, the next steps are to (1) obtain the modeling system (if you are reading this user's guide we assume that you have already done this and have visited our REMSAD web site at http://remsad.saintl.com), (2) design and set up the REMSAD application, (3) identify/allocate sufficient computer resources, and (4) conduct the modeling exercise. Information provided in this section is intended to help new users to understand and conduct these general tasks.

3.1. Key Considerations in the Design and Set Up of a REMSAD Application

New or first-time users of the REMSAD modeling system will have a lot to do to prepare for modeling. Things will go more smoothly if some time is devoted beforehand to the careful design of the modeling exercise.

First and foremost, the user should clearly identify the objective(s) of the REMSAD modeling exercise. The objective(s) may range from completing a graduate-degree program involving the assessment of some aspect of the modeling system, to evaluating the ability of REMSAD to replicate observed data, to developing a regional-scale air quality management program for regional haze. Clearly defined objective(s) will support subsequent decision-making regarding the level of detail and effort required for the application.

In designing a REMSAD modeling analysis, some of the key considerations include:

- *Modeling domain specification.* The REMSAD modeling domain should be designed such that the horizontal and vertical extent minimizes the potential influence of the boundary conditions (which cannot be known) on the simulation results for the area(s) of interest. This influence may vary according to species of interest and meteorological conditions. Other factors to consider, that tend to put limitations on the size of the modeling domain, include the availability of input data or databases to support the model application and the conflicting constraints of grid resolution and computational resources. It is a good idea to perform numerical tests (or sensitivity simulations) to examine the influence of the boundary conditions on the simulation results for the areas of interest, before finalizing the modeling domain.

  The horizontal and vertical resolution of the domain may affect the ability of the model to realistically represent the relevant atmospheric processes and observed concentrations. Grid resolution may also influence the response of the modeling system to changes in emissions. The nested-grid feature of REMSAD is designed to accommodate higher resolution where needed or desired, without the computational burden that would be associated with that same resolution throughout the domain. REMSAD-based, national-scale analyses of air quality issues for the U.S. have typically used 56 to 36 km horizontal resolution. More refined analyses have included higher resolution nested grids (typically 12 km) over key regions or areas of interest.

REMSAD has typically been exercised with 8 to 15 layers extending to approximately 10,000 m agl. These layers are specified such that the highest resolution is achieved near the surface.

Two examples of a REMSAD modeling domain are presented in Figure 3-1. In both cases, the modeling domain relies on an outer coarse grid with 36 km resolution; one or more nested grids are also included.

Figure 3-1a
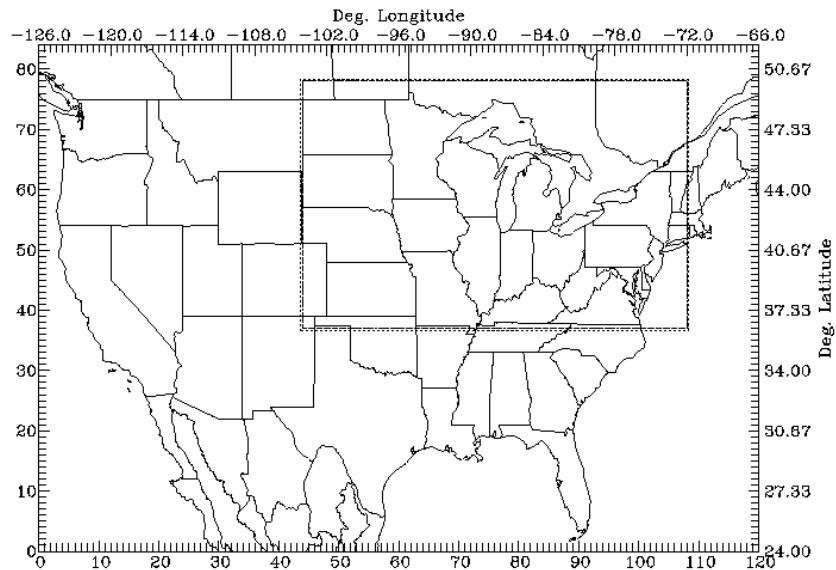
Figure 3-1b
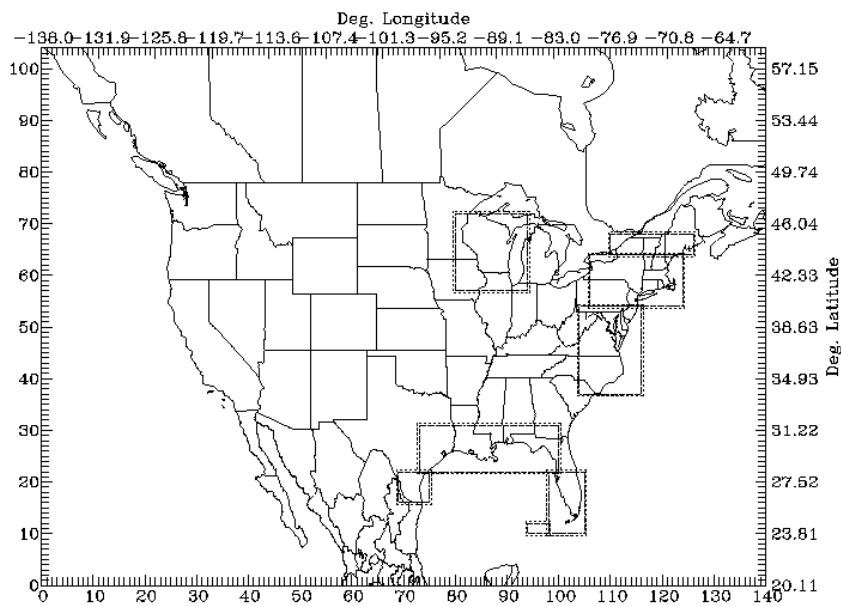
- *Modeling period.* REMSAD is designed for annual applications, but can be applied to shorter or longer periods as well. The availability of existing input databases (e.g., meteorological and emission inputs) may pre-determine the simulation period. Otherwise, it is recommended that the simulation period be selected to be representative of the meteorological and air quality conditions that characterize or exemplify the air quality issue being addressed. In addition, the availability of data for the evaluation of model performance (e.g., some data may be only available as seasonal or annual summaries) as well as the period of interest for certain air quality standards or goals (e.g., annual standard for $PM_{2.5}$) may also guide the selection of the modeling period.

- *Input preparation procedures.* As described in the following section of this user's guide, there are many options available for the preparation of inputs for REMSAD. A consistent and reliable set of methodologies for preparing the inputs should be identified that support the level of detail required for the application. The input preparation procedures should address the preparation of the requisite meteorological, emissions, boundary condition, and geographic inputs. Certain of the input files, such as the chemistry parameter file, are specific to the chemical mechanism and should not be changed. The input files are discussed in more detail in the following section.

- *Chemistry options.* REMSAD supports the use of parameterized or micro-CB gas-phase chemistry. Use of the micro-CB-IV chemistry is recommended for all applications.

- *Simulation and output species.* Depending on the focus of your application, it may not be important or necessary to simulate or save (to output) certain of the REMSAD species. For PM only applications, for example, you may choose to not simulate the toxic species. Refining the list of species to simulate and output will help to define (and, as needed, minimize) the computer requirements for the application.

- *Model performance evaluation.* Model performance evaluation methods and expectations regarding what constitutes acceptable model performance should be established prior to commencing with the application. EPA (2000) provides suggestions on model performance metrics and criteria as related to the use of model to demonstrate attainment of air quality goals for $PM_{2.5}$ and regional haze. These may also provide a starting point for other types of applications. The methods and expectations should be designed to ensure confidence in the results relative to how they will be used to further research or air quality planning objectives.

- *Computer resource requirements.* The availability of computer resources relative to the intended schedule for the modeling exercise should be considered, especially in specifying the modeling domain and simulation period. Some additional information on computer system requirements is provided next.

3.2. Computer System Requirements

The computer memory and CPU time requirements will be determined by the number of grid cells (in the horizontal and vertical; including nested grids), grid resolution, and length of the simulation period. Disk storage requirements will be determined by the number of grid cells (including nested grid), the length of the simulation period, and the number of output species. Table 3-1 provides the CPU and disk storage requirements for three recent REMSAD simulations of varying complexity. These simulations were run on a Compaq/DEC Alpha XP1000 workstation with a single 677 MHz CPU and 2 GB RAM. This table is intended to provide some benchmark storage and CPU requirements as well as a basis for comparing and

qualitatively assessing the requirements for new simulations and/or other computer systems. The run times given in this table are based on the use of the micro-CB chemistry.

Do any of the parameters given in Table 3-1 need to change for Version 7.

Table 3-1.
Computer storage (disk space), memory, and CPU requirements
for three example REMSAD applications.

Domain	Continental U.S.	Continental U.S. (with 1 nested grid)	Continental U.S. (with 8 nested grids)
Coarse-grid resolution (km)	36	36	36
Number of nested grids	0	1	8
Resolution of nested grid(s) (km)	NA	12	12
Total number of horizontal grid cells	10,080	31,072	24,927
Number of vertical layers	12	12	15
Total number of grid cells	110,880	341,792	373,905
Number of output species	28	28	27
Time interval for the input files (hr)	1	1	3
Emissions specified for nested grid(s)	NA	Yes	Yes
Meteorological inputs specified for nested grids	NA	No	No
Disk storage requirement for input files per simulation day (mbytes)	120	125	53
Disk storage requirement for input files per year (mbytes)	38,000	40,000	20,000
Disk storage requirements for output files per day (mbytes)	170	790	200
Disk storage requirements for output files per year (mbytes)	62,000	290,000	73,000
Total disk storage requirements per day (mbytes)	290	915	169
Total disk storage requirements per year (mbytes)	106,000	330,000	62,000
Memory requirement (mbytes)	1,000	1,000	1,000
Run time requirement per day (hrs)	1.3	3.8	1.7
Run time requirement per year (hrs)	475	1275	620

3.3. Step-by-Step Summary of REMSAD Application Procedures

The general application procedures for REMSAD follow those for most other air quality models as depicted in Figure 3-2.

REMSAD also offers an alternative application procedure that entails running the simulation in two parts, when mercury or other toxic species are considered. This is also depicted in Figure 3-2. Because the interaction between the criteria pollutants and the toxic species is largely one-way, the toxic species can be simulated separately. In this case, the criteria pollutants are simulated first and detailed, hourly (or 3-hour outputs) are saved for later use. The toxic-species-only simulation is then conducted separately. The run time and disk storage requirements for the toxic-species-only simulation are much less than for the full criteria pollutant simulation (refer to Table 3-1). For example, for a simulation for the domain with one nested grid, the run time is 2.8 hrs CPU per simulation day for the criteria pollutant simulation and 1.0 hrs CPU for the mercury simulation. The motivation for conducting the simulation in two parts is that sensitivity simulations involving toxic species only (e.g., use of different tags for mercury species, or changes in mercury emissions speciation) can then be more quickly and easily run.

Figure 3-2.
Typical REMSAD application procedure.
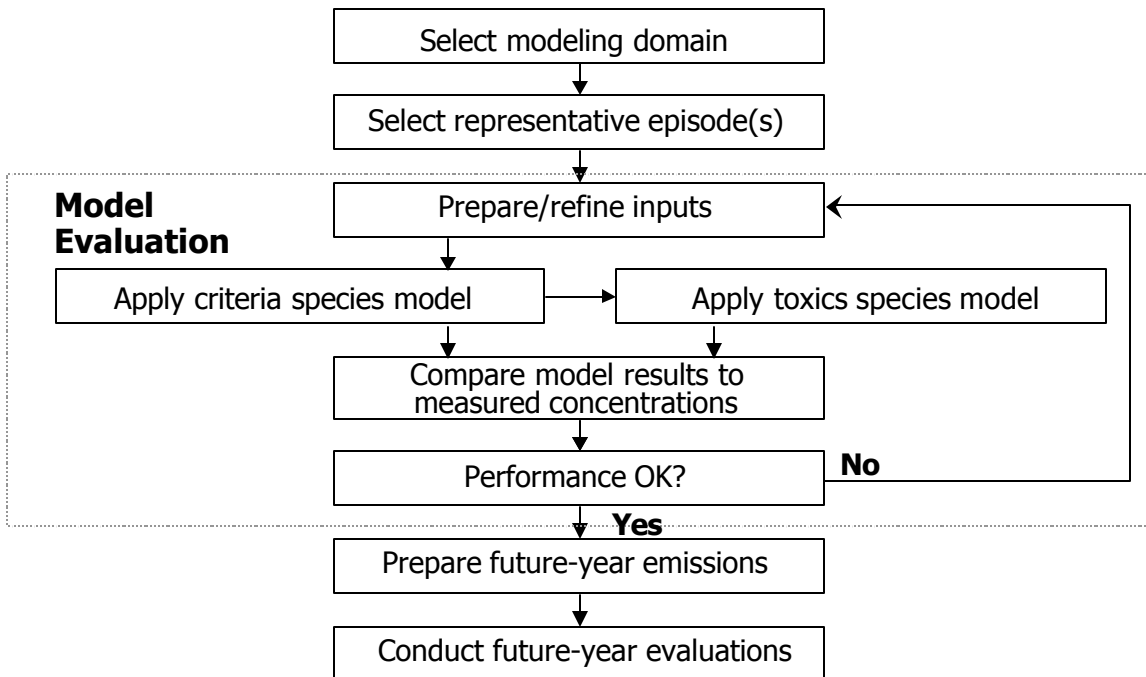
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4. REMSAD INPUT REQUIREMENTS AND PREPARATION PROCEDURES

REMSAD requires a variety of input files that characterize and describe the emissions, meteorological conditions, initial and boundary species concentrations, geographical and land-use features, and chemistry parameters corresponding to the modeling domain and simulation period. These inputs provide the basis for the air quality calculations. The input files and preparation procedures are described in this section of the user's guide.

For ease of reading, many of the larger (file format information) exhibits follow the text of this section.

4.1. Summary of Input File Requirements

There are seventeen input files for REMSAD. These fall into the general categories of emissions, initial and boundary conditions, meteorological fields, surface characteristics, chemical parameters, and simulation control parameters. The files are listed and briefly described in Table 4-1. The units required for each type of input are also listed (where appropriate). Several of the files consist of two- or three-dimensional fields of the input variables and this is indicated in the table. In additional, several of the files contain information that varies with time (according to the input time interval selected for the REMSAD application—typically 1 to 3 hours). This is also indicated in the summary table.

Table 4-1
Summary of REMSAD input files.

File Type/Name	Description	Units	2-D	3-D	Time Variant
Emissions					
EMISSIONS	Low-level emissions for area, mobile, low-level point, non-road, and biogenic sources	Moles/hr (gaseous) Grams/hr (particulates)	✔		✔
PTSOURCE	Elevated point-source emissions	Moles/hr (gaseous) Grams/hr (particulates)			✔
Initial and Boundary Conditions					
AIRQUALITY	Initial species concentrations for each grid cell within the modeling domain	ppm, or μg/(mole air) *See note 1*		✔	
BOUNDARY	Species concentrations along the lateral boundaries of the modeling domain	ppm or μg/(mole air) *See note 1*	✔ *See note 2*		✔
CHLORINE	Surface chlorine concentrations	ppt	✔		

File Type/Name	Description	Units	2-D	3-D	Time Variant
Meteorological Fields					
WIND	u- and v- wind components	ms^{-1}		✓	✓
TEMPERATURE	Temperature	K		✓	✓
PSURF	Surface Pressure	Mb	✓		✓
H2O	Water vapor concentration	kg water/kg air		✓	✓
VDIFFUSION	Vertical diffusivities or exchange coefficients	m^{2}s^{-1}		✓	✓
CLW	Cloud-water mixing ratio	kg water/kg air		✓	✓
RLW	Rain-water mixing ratio	kg water/kg air		✓	✓
RAIN	Rainfall rate	in/hr	✓		✓
Surface Characteristics					
SURFACE	Land-use characteristics	NA; given as fraction of grid cell	✓		
TERRAIN	Terrain heights	M	✓ *See note 3*		
Chemistry Parameters					
CHEMPARAM	Chemical reaction rates and other micro-CB parameters	Various			
RATES	Photolysis rates	min^{-1}			
Simulation Control					
SIMCONTROL		NA			

Note 1: Boundary conditions units are ppm for all species except SOA, POA, PEC, PMFINE, and PMCOARS. For SOA, POA, PEC, PMFINE, and PMCOARSE the units are μg/(mole air).

Note 2: Boundary concentrations consist of a two dimensional array of values (layers by horizontal dimension, either x or y) for each of the four sides of the domain.

Note 3: Use of all zero terrain heights is currently recommended which has the effect of making photolysis rate estimates to be taken at height above ground rather than above sea level.

Many of the REMSAD input files are unformatted, binary files that have a similar file structure. These files include three types of records: header records, time-invariant records, and time-varying records.

- *Header records* consist of up to four records. The first line contains the file description information, which includes a specific file name, an optional file identifier, and the number of chemical species. The second record contains information about the modeling domain including the geographical[1] coordinates of the origin of the domain, grid cell size in the x-

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1 REMSAD is intended for regional-scale applications for which the most appropriate coordinates are latitude and longitude or Lambert conformal.

and y- directions, the number of grid cells in the x- and y- directions, and the number of vertical layers. The third record is the segment description record. REMSAD does not support segmented simulation; only one segment (corresponding to the entire modeling domain) is defined by the x- and y-location of the segment offset from the modeling region (must be 0) and the number of grid cells along the x and y axes. The final record contains the species name for each species (corresponding to the number of species given on the file description record). The meteorological and land use files do not contain header records.

- *Time-invariant records* contain information for data that do not vary with time, e.g., terrain height. The types of data vary from file to file.

- *Time-varying records* contain information for data that do vary with time, e.g., temperature. The types of data vary from file to file.

Several of the REMSAD input files are formatted, ASCII files. These include the chemistry parameters, photlysis rates, chlorine concentrations, and simulation control files.

In the remainder of this section, each of the REMSAD input files is described further with emphasis on file content, file format, use in the modeling system, and suggested preparation procedures. Not all files are needed for all simulations (some files are optional) and all grids (some files are specified for the coarse-grid only or are optional for the fine grids). This information is also provided in the following discussion.

4.2. Emissions

There are two types of emissions files. The low-level or EMISSIONS file contains emissions that are emitted within the lowest or surface-based layer of the REMSAD model. The low-level emissions are comprised of emissions from area (e.g., emissions associated with home-heating equipment, dry cleaning and solvent use, agricultural processes (including burning), and meat cooking), mobile, low-level point, and biogenic sources. The PTSOURCE file contains emissions from elevated point sources. For criteria pollutants the emissions inventory should contain emissions for the following species: nitric oxide (NO), nitrogen dioxide (NO_2), primary organic aerosols (POA), primary elemental carbon (PEC), gaseous pathway sulfate particles (GSO4), particulate nitrate (PNO3), volatile organic compounds (VOC), secondary organic aerosols (SOA), sulfur dioxide (SO2), fine particulates (PMFINE), coarse particulates (PMCOARS), ammonia (NH3), carbon monoxide (CO), carbonyl (CARB), and isoprene (ISOP).

CARB is included in micro-CB-IV in recognition of the fact that many photochemically reactive hydrocarbons decay to a carbonyl species (formaldehyde, acetaldehyde, ketones, or in some cases a higher aldehyde). The carbonyl species thus formed participate further in the photochemistry. The CARB species, formed from reactions involving the VOC species in REMSAD, therefore allows a representation of these secondary carbonyl species. Although most of the CARB that appears in simulations is a product of the VOC reactions, some carbonyls are emitted directly and it is therefore appropriate to include some CARB in the emissions. Up to this point CARB has been introduced into the emissions at a constant percentage of the VOC emissions (in the range of 3 to 7%). Our current recommendation is to use a constant fraction 3% of VOC as CARB, which is believed to perform adequately in comparison to the full CB-IV. For Version 7, the species TOL and XYL may be included in the EMISSIONS file in order to facilitate the estimation of the aromatic fraction in the emissions. The aromatic fraction is used in calculating the yield of SOA from the gas phase photochemistry. TOL and XYL are not explicitly used in the chemical mechanism and their

inclusion will not affect any process other than SOA formation. When TOL and XYL are included, the emissions of VOC and CARB should not be modified. For further information, see the section on the SOA treatment.

ISOP and TERP represent biogenic emissions in REMSAD and should be calculated from species produced by biogenic processors such as BEIS2 as follows: ISOP = isoprene + (10/5)*(other VOC)/3; TERP = monoterpenes. This calculation assumes that all species are expressed in moles. ISOP and TERP are the micro-CB species, "isoprene" is the isoprene estimated by BEIS2, "monoterpenes" is the amount estimated by BEIS2, and "other VOC" is other biogenic emissions estimated by BEIS2 that are not assigned to a specific species group. The factor 10/5 corrects for carbon number (monoterpenes and other VOC are treated as 10 carbon molecules by BEIS2, ISOP and isoprene are 5 carbon molecules) and the factor of 3 is a reactivity correction to account for differences in isoprene and other biogenic emission reactivity. TERP is also a 10 carbon molecule and is set directly to the mass of monoterpenes.

Emissions of mercury and other toxic species must also be specified in the appropriate emissions files (either with or separate from the criteria pollutant emissions). Since REMSAD accounts for spatial and temporal variations as well as reactivity differences (i.e., chemical composition) of the emissions, the input emissions data must contain a comparable level of resolution. The standard REMSAD species are listed in Table 4-2.

TABLE 4-2.
REMSAD emissions species for a typical REMSAD application.

REMSAD (Version 7) Emissions Species	Species ID	Units
Nitric oxide	NO	moles/hr
Nitrogen dioxide	NO2	moles/hr
Primary organic aerosols	POA	gm/hr
Primary elemental carbon	PEC	gm/hr
Gaseous sulfate	GSO4	gm/hr
Particulate nitrate	PNO3	gm/hr
Volatile organic carbon	VOC	moles/hr
Toluene (optional)	TOL	moles/hr
Xylene (optional)	XYL	moles/hr
Secondary organic aerosols	SOA	gm/hr
Sulfur dioxide	SO2	moles/hr
Particulate matter with a diameter less than 2.5 microns	PMFINE	gm/hr
Particulate matter with a diameter greater than 2.5 but less than 10 microns	PMCOARS	gm/hr
Ammonia	NH3	moles/hr
Carbon monoxide	CO	moles/hr
Carbonyl	CARB	moles/hr

REMSAD (Version 7) Emissions Species	Species ID	Units
Isoprene	ISOP	moles/hr
Monoterpenes	TERP	moles/hr
Mercury—elemental	HG0	moles/hr
Mercury—divalent	HG2	moles/hr
Mercury—particulate	HGP	gm/hr

The REMSAD emissions files can be prepared using a variety of emission processing software, provided that the content and format of the file are matched to the requirements of REMSAD. To date, most of the emission inventories for REMSAD applications have been prepared using an enhanced version of the Emissions Preprocessing System (EPS2.5). Additional information on EPS2.5 can be found on the REMSAD web site (http://remsad.saintl.com). Biogenic emissions can be estimated using the Biogenic Emission Inventory System (BEIS-2).

4.2.1. Low-Level Emissions (EMISSIONS)

Total emission rates for low-level sources for each grid cell, species, and update interval are provided in the EMISSIONS file. The EMISSIONS file contains total emission rates for each emitted species at each horizontal grid location from a combination of area, mobile, low-level point, and biogenic sources. The units for the emissions in this file are moles per hour for gaseous species and grams per hour for particulates.

EMISSIONS files must be provided for the coarse grid and each nested grid. EMISSIONS files for the nested grids cover all grid cells of the nested grid system including boundary cells (as discussed later in this section).

Typically three EMISSIONS files are provided for each grid, representing weekday, Saturday, and Sunday emissions. The L1EDAY flag in the simulation control file (discussed later in this section) enables the use of generic weekday, Saturday, and Sunday emissions (i.e., the date on the file does not have to match that for the simulation). If it is not possible to distinguish weekday and weekend emissions, the same EMISSIONS file can be used for all days of the simulation.

The format and record structure of the EMISSIONS file is shown in Exhibit 4-1.

4.2.2. Point Sources (PTSOURCE)

For each point source located within the domain, the following information must be specified: location, stack height, stack diameter, stack exit temperature, stack exit velocity, and emission rates for all species. Emission rates for each point source for each emitted species can optionally be specified separately for each update interval. The units for the emissions in this file are moles per hour for gaseous species and grams per hour for particulates.

The PTSOURCE file contains the following information for each designated "point source."

- Location.

- Stack parameters (height, diameter, exhaust temperature, flow rate).

- Emissions for each species as required by chemical mechanism.

A single PTSOURCE file is provided for the coarse grid; files need not be specified for fine grids. REMSAD calculates the location of each source within the appropriate grid.

Note that the REMSAD program currently calculates plume rise during simulation and the point source emissions are added directly to the corresponding grid cell.

The format and record structure of the PTSOURCE file is shown in Exhibit 4-2.

4.2.3.   Initial and Boundary Concentrations

There are two REMSAD air quality input files that define pollutant concentrations for each of the REMSAD state species (1) throughout the three-dimensional grid at the initial simulation time (coarse-grid only), and (2) along the lateral boundaries of the modeling domain for each hour of the simulation period. A default concentration value of 1×10^{-20} ppm is assigned to any modeled species not directly specified in the initial and boundary condition files. This default value is also applied to concentrations of all species at the top of the modeling domain.

The REMSAD modeling system includes preprocessor programs for the preparation of the initial and boundary condition files.

4.2.4.   Initial Concentrations (AIRQUALITY)

The AIRQUALITY file contains the initial concentration in parts per million (ppm) for each simulated species, with the exception SOA, POA, PEC, PMFINE, and PMCOARS, for each grid cell. The units for SOA, POA, PEC, PMFINE, and PMCOARS are μg/(mole air). It is required for the coarse grid only.

Initial concentrations can be uniform or can vary in the horizontal and vertical. The AIRQUALITY file can be generated using the AIRQUL preprocessor program or using other techniques. The AIRQUL preprocessor program is also a component of the UAM-V modeling system and is available on the REMSAD web site (http://remsad.saintl.com).

The format and record structure of the AIRQUALITY file is shown in Exhibit 4-3a. An example input file for the AIRQUL preprocessor program is shown in Exhibit 4-3b. Note that in this example a UNITS packet is included in the preprocessor inputs. The UNITS packet lists species whose concentrations as provided in the preprocessor inputs are to be converted from ppb to ppm prior to writing the values to the data file. The concentration values on the binary AIRQUALITY file should always be ppm (or μg/(mole air) as specified in Exhibit 4-3a.

4.2.5.   Lateral Boundary Concentrations (BOUNDARY)

The BOUNDARY file defines the boundary of the REMSAD coarse-grid domain as well as the hourly (or update interval) concentration in parts per million of each species, with the exception SOA, POA, PEC, PMFINE, and PMCOARS, for each lateral boundary cell on the coarse grid. The units for SOA, POA, PEC, PMFINE, and PMCOARS are μg/(mole air). The BOUNDARY file also may be used to exclude specified groups of outlying coarse-grid cells from REMSAD calculations. The defined boundaries must not intersect a nested grid area. Lateral boundary concentrations can vary in space and time. The units for all species are ppm.

Boundary conditions are required for the calculation of the advective transport term at grid cells adjacent to lateral boundaries, when the corresponding wind component is directed into the domain.

The BOUNDARY file can be generated using the BOUNDARY preprocessor program or using other techniques. The BOUNDARY preprocessor program is also a component of the UAM-V modeling system and is available on the REMSAD web site (http://remsad.saintl.com).

The format and record structure of the BOUNDARY file is shown in Exhibit 4-4a. An example input file for the BOUNDARY preprocessor program is shown in Exhibit 4-4b. In this example, as in the example for AIRQUALITY, a UNITS packet is included in the preprocessor inputs. The UNITS packet lists species whose concentrations as provided in the preprocessor inputs are to be converted from ppb to ppm prior to writing the values to the data file. The concentration values on the binary BOUNDARY file should always be ppm (or µg/(mole air) as specified in Exhibit 4-4a.

4.2.6.   Chlorine Concentrations

The CHLORINE file contains the surface concentrations of chlorine (Cl_2) in ppt. A value of the chlorine concentration must be provided for each grid cell in the coarse grid modeling domain. This file must be provided with a value for each grid cell in all simulations, but the data value is only used in the mercury chemistry routine. Hence, for a simulation that does not include mercury, this file can be a dummy file containing the same value for all grid cells.

Our current recommendation for the chlorine concentrations is a value of 125 ppt over the ocean and up to 100 km inland. Over land, the recommended value is 5 ppt. Within the model, chlorine concentrations are linearly interpolated between the surface value and zero at an altitude of 1000 m over land and 2000 m over the ocean. The chlorine concentration is set to zero during daylight hours within the model.

The chlorine concentration file is an ASCII file that must include one line in the file for each coarse grid cell in the domain. The input lines are free formatted and contain the x-grid cell index, the y-grid cell index, and the chlorine concentration in ppt. A sample of a portion of the chlorine file is shown below.

```
1 1 125
1 2 125
1 3 125
1 4 125
1 5 125
1 6 125
1 7 125
1 8 125
1 9 125
1 10 125
1 11 125
1 12 125
1 13 125
1 14 125
…
9 94 125
9 95 125
9 96 125
9 97 5
```

```
9 98 5
9 99 5
9 100 5
9 101 5
9 102 5
9 103 5
9 104 5
10 1 125
10 2 125
10 3 125
10 4 125
…
```

4.3. Meteorological Inputs

Meteorological inputs required by Version 7 of the REMSAD modeling system include gridded fields of wind, temperature, surface pressure, water vapor concentration, vertical exchange coefficient, cloud cover, cloud-water mixing ratio, rainfall rate, and liquid-water mixing ratio. All meteorological variables are specified for each grid cell of the modeling domain. All of these inputs can be obtained or derived from output from dynamic meteorological models. Most applications of REMSAD to date have used meteorological inputs derived from either the Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR) Mesoscale Model (MM5 or, in some cases, MM4)), or the Rapid Update Cycle (RUC) modeling system (developed and operated by NOAA/OAR/FSL/FDR).

4.3.1. Wind (WIND)

The WIND file contains the horizontal wind components (u and v) for each grid cell for each hour (or update interval) of the simulation. The vertical (w) wind component is not an input; instead it is calculated by REMSAD from the horizontal wind inputs. The units for the wind components are ms^{-1}.

The wind fields determine the transport of simulated pollutants. The u and v components are used to evaluate the horizontal advection terms in the advection/diffusion equation, calculate vertical velocities, calculate surface layer parameters for deposition, determine plume rise characteristics, and diagnose diffusion coefficients.

As noted above, wind fields are usually derived from the output of a meteorological model. The output from the meteorological model must be mapped to the REMSAD grid (and converted to the units and formats required by REMSAD). The horizontal wind components (u and v) must be specified for one of two optional configurations: winds at each grid cell center, or winds staggered to horizontal grid cell interfaces. For example, both the MM5 and RUC model output wind components are staggered in the horizontal and thus the staggered option is typically employed when using output from these meteorological models.

A WIND file must be supplied for the coarse grid. WIND files may also be supplied for any nested grids. If no WIND file is supplied for a nested grid, the values for that grid are interpolated from the coarse grid.

The WIND file is a binary, unformatted file that has a maximum record length equal to the number of grid cells in the x-direction times the number of grid cells in the y-direction. The format and record structure of the WIND file is shown in Exhibit 4-5.

4.3.2. Temperature (TEMPERATURE)

The TEMPERATURE file defines the absolute temperature for each grid cell for each hour (or update interval) of the simulation. The temperature must be specified at the center of each grid cell. The units for temperature are Kelvins (K).

Temperature information is necessary to evaluate certain reaction rates within the chemistry module, and to determine plume rise characteristics. Surface temperature is used for the dry deposition calculation.

As noted above, temperature fields are usually derived from the output of a meteorological model. The output from the meteorological model must be mapped to the REMSAD grid (and converted to the units and formats required by REMSAD).

A TEMPERATURE file must be supplied for the coarse grid. The coarse-grid temperatures are interpolated to any nested fine grid by REMSAD.

The TEMPERATURE file is a binary, unformatted file that has a maximum record length equal to the number of grid cells in the x-direction times the number of grid cells in the y-direction. The format and record structure of the TEMPERATURE file is shown in Exhibit 4-6.

4.3.3. Surface Pressure (PSURF)

The surface pressure file contains the surface pressure in millibars (mb). Surface pressure is specified for each grid cell for each hour (or update interval) of the simulation.

Surface pressure is used to define the vertical layer structure within the sigma (σ) coordinate system as well as the pressure at the center of each grid cell. The surface pressure in combination with the terrain elevation is also used to define the height of each layer interface for each cell column. Height and pressure are subsequently used to determine altitude-dependent photolysis rates, pressure dependent rate constants, internal mass-concentration conversions, and stability for surface deposition and plume rise.

Gridded fields of surface pressure are usually derived from the output of a meteorological model. The output from the meteorological model must be mapped to the REMSAD grid (and converted to the units and formats required by REMSAD). Surface pressure is given for the center of the grid cell.

Surface pressure is specified for each coarse-grid cell and optionally for each fine-grid cell. Surface pressure is specified for the lowest model layer only.

The PSURF file is a binary, unformatted file that has a maximum record length equal to the number of grid cells in the x-direction times the number of grid cells in the y-direction. The format and record structure of the PSURF file is shown in Exhibit 4-7.

4.3.4. Water Vapor (H2O)

The H2O file contains the concentration of water vapor in kg of water per kg of air and is therefore a unitless number. Water vapor concentration is specified for each grid cell for each hour (or update interval) of the simulation. This is one of several moisture variables required by REMSAD.

Water vapor concentration is necessary for evaluation of certain reaction rates within the chemistry module.

Water vapor concentration fields are usually derived from the output of a meteorological model. The output from the meteorological model must be mapped to the REMSAD grid (and converted to the units and formats required by REMSAD). The concentration of water vapor must be specified hourly (or for each update interval) at the center of each grid cell.

An H2O file must be supplied for the coarse grid. The coarse-grid water-vapor concentrations are interpolated to any nested fine grid by REMSAD.

The H2O file is a binary, unformatted file that has a maximum record length equal to the number of grid cells in the x-direction times the number of grid cells in the y-direction. The format and record structure of the H2O file is shown in Exhibit 4-8.

4.3.5. Vertical Turbulent Exchange Coefficients (K_v) (VDIFFUSION)

The VDIFFUSION file contains gridded vertical turbulent exchange coefficients (or diffusivities) for each hour (or update interval) of the simulation period. The units for the vertical exchange coefficients (or K_vs) are m^2s^{-1}.

The vertical exchange coefficients are used to estimate the mixing of pollutants between two adjacent layers due to subgrid-scale turbulent diffusion (eddy diffusivity). The vertical profile of Kv also determines the effective mixing height within each REMSAD modeling grid column. Among the meteorological inputs, this is one of the more important, and the simulation results can be very sensitive to the specification of this parameter.

K_v fields for REMSAD are usually derived from the output of a meteorological model, using one of the following approaches. In the first approach, the K_vs can be obtained directly from the meteorological model. This same variable is used to simulate the turbulent exchange of momentum and heat properties within most dynamic meteorological modeling systems. The second approach is to calculate K_v using meteorological-model-derived estimates of turbulent kinetic energy (TKE). Formulas such as those provided by Garratt (1992) provide the necessary relationships. The third approach is to diagnose K_v from the wind, temperature, and pressure fields. This diagnostic approach is based on the estimation of local stability as characterized by the Richardson number. Based on stability, different empirical formulas are used to estimate the K_vs. The K_vs must be specified at the top of each grid cell (i.e., at the layer interface of each grid cell).

A VDIFFUSION file must be supplied for the coarse grid. VDIFFUSION files may also be supplied for any nested grids. If no VDIFFUSION file is supplied for a nested grid, the values for that grid are interpolated from the coarse grid.

The VDIFFUSION file is a binary, unformatted file that has a maximum record length equal to the number of grid cells in the x-direction times the number of grid cells in the y-direction. The format and record structure of the VDIFFUSION file is shown in Exhibit 4-9.

4.3.6. Cloud Liquid Water Mixing Ratio (CLW)

The CLW file contains the mixing ratio (or the mass of liquid water (in kilograms) per kilogram of dry air within a cloud) that describes the liquid water content of clouds when present in a grid cell. Cloud liquid water mixing ratio is specified for each grid cell and hour (or update interval) of

the simulation. This is a dimensionless variable and one of several moisture variables required by REMSAD.

Cloud liquid water mixing ratio is used specifically to determine the reaction rates involved in the REMSAD aqueous-phase chemistry (pertaining to sulfate formation and mercury chemistry). It is also used in determining wet deposition rates.

Cloud liquid water mixing ratio is usually derived from the output of a meteorological model. The output from the meteorological model must be mapped to the REMSAD grid (and converted to the units and formats required by REMSAD). The cloud water mixing ratio must be specified at the center of each grid cell.

A CLW file must be supplied for the coarse grid. The coarse-grid cloud liquid water mixing ratio values are interpolated to any nested fine grid by REMSAD.

The CLW file is a binary, unformatted file that has a maximum record length equal to the number of grid cells in the x-direction times the number of grid cells in the y-direction. The format and record structure of the CLW file is shown in Exhibit 4-10.

4.3.7.   Rain Liquid Water Mixing Ratio (RLW)

The RLW file contains the mixing ratio (or the mass of liquid water (in kilograms) per kilogram of dry air within a precipitating air mass) that describes the liquid water content of rain when present in a grid cell. Rain liquid water mixing ratio is specified for each grid cell and hour (or update interval) of the simulation. This is a dimensionless variable and one of several moisture variables required by REMSAD.

Rain liquid water mixing ratio is used specifically to determine wet deposition rates of the simulated species. Cloud liquid water mixing ratio and rain liquid water mixing ratio in combination determine the amount of liquid water present for gaseous species to dissolve in.

Rain liquid water mixing ratio is usually derived from the output of a meteorological model. The output from the meteorological model must be mapped to the REMSAD grid (and converted to the units and formats required by REMSAD). The rain water mixing ratio must be specified at the center of each grid cell.

An RLW file must be supplied for the coarse grid. The coarse-grid rain liquid water mixing ration values are interpolated to any nested fine grid by REMSAD.

The RLW file is a binary, unformatted file that has a maximum record length equal to the number of grid cells in the x-direction times the number of grid cells in the y- direction. The format and record structure of the RLW file is shown in Exhibit 4-11.

4.3.8.   Precipitation Rates (RAIN)

The RAIN file provides hourly (or update interval specific) rainfall rates for each horizontal grid cell. This is an option file for REMSAD, but is required for the calculation of wet deposition. The units are in/hr.

Rainfall rate is used to calculate the net removal of gases and aerosols by rain scavenging through the depth of each model column.

Rainfall rates are usually derived from the output of a meteorological model. The output from the meteorological model must be mapped to the REMSAD grid (and converted to the units and formats required by REMSAD). The rainfall rate is specified to represent the entire grid cell.

A RAIN file is provided for the coarse grid only. The coarse-grid rain liquid water mixing ratio values are interpolated to any nested fine grid by REMSAD.

The RAIN file is a binary, unformatted file that has a maximum record length equal to the number of grid cells in the x-direction times the number of grid cells in the y-direction. The format and record structure of the RAIN file is shown in Exhibit 4-12.

4.4. Surface Characteristics

4.4.1. Land Use (SURFACE)

The surface characteristics file contains the distribution of land-use types for each horizontal grid cell. This is given as fraction of each REMSAD land-use category for each grid cell. The land-use categories employed by REMSAD and the associated roughness lengths are listed in Table 4-3.

Table 4-3.
Land-use categories recognized by REMSAD.

Category Number	Land-Use Category	Surface Roughness (meters)
1	Urban	3.00
2	Agricultural	0.25
3	Range	0.05
4	Deciduous forest	1.00
5	Coniferous forest including wetland	1.00
6	Mixed forest	1.00
7	Water	0.0001
8	Barren land	0.002
9	Nonforest wetlands	0.15
10	Mixed agricultural and range	0.10
11	Rocky (low shrubs)	0.10

Land-use type determines the UV albedo, roughness length, and surface resistance to deposition for gaseous species.

For application of REMSAD for the U.S., land-use inputs are generally extracted from a U.S. Geological Survey (USGS) land-use database. Surface characteristics may vary spatially but not temporally.

A SURFACE file must be provided for the outer (coarse) grid and may be (optionally) provided for any nested grids. If a SURFACE file is not provided, data from the coarse-grid file are interpolated to each nested grid.

The SURFACE file is a binary, unformatted data file. The format and record structure of the SURFACE file is shown in Exhibit 4-13.

4.4.2. Terrain Height Definition (TERRAIN)

This file contains elevation (above sea level) of the ground surface of each horizontal grid cell.

This version of REMSAD does not require specification of terrain heights and users should simply supply a file with all terrain heights set equal to zero. Although not used in the current version of REMSAD, we retain this file in the event that future updates or additions to the model require terrain data. Please note that the influence of terrain on the advection/diffusion processes is communicated to REMSAD through the meteorological inputs.

A TERRAIN file must be provided for the outer (coarse) grid.

The TERRAIN file is a binary, unformatted data file. The format and record structure of the SURFACE file is shown in Exhibit 4-14.

4.5. Chemical Reaction and Photolysis Rates

Application of the REMSAD modeling system requires preparation of several additional input files that contain information on chemical reaction rates, particle size and mass distribution, and photolysis rates. The chemical reaction variables should not be altered for individual applications; rather, they are only changed during upgrades to the chemical mechanism.

4.5.1. Chemistry Parameters (CHEMPARAM)

The CHEMPARAM file contains information regarding the chemical species to be simulated. For gas-phase species chemistry parameters determine the rates and temperature dependence for the gas-phase reactions and include chemical reaction rates, activation energies, and maximum/minimum species concentrations. For particulate species, the parameters include particle size and mass distribution, particle density, and hydroscopic affinity factor.

The chemistry parameter file is provided with REMSAD; it should be modified to reflect the species included in the simulation (e.g., for inclusion of toxic species). The parameters are specific to the version of REMSAD and should not be modified. Particle size and mass distribution are fixed for the parameterization used in REMSAD. These numbers should not be altered. Mass distributions are fractions of mass in each of the size ranges. These distributions are assigned based on the expected distribution of the particulate component. For example, the value following the species name GSO4 is a 2 indicating mass distribution 2, which is skewed towards fine particle size ranges. This is consistent with the processes that form GSO4 which are gas phase processes. Other species such as PMFINE and PMCOARS use distinctly separate size ranges since they are designed to differentiate fine and coarse particulate emissions. NH4N and NH4S do not reference a size distribution because they are tied to the distributions for PNO3 and ASO4, respectively. The size distributions are used in the wet and dry deposition algorithms in order to incorporate effects that are dependent on particle size (e.g., sedimentation velocity, washout).

A standard CHEMPARAM file for REMSAD, version 7 with micro-CB chemistry is provided in Exhibit 4-15.

4.5.2. Photolysis Rates (RATES)

The RATES file contains tabulated photolysis rates for five key reactions: photolysis of NO_2, HCHO (two product channels), O_3 (to form $O(^1D)$) and ALD2. The rates of these reactions are function of height and solar zenith angle under constant albedo, ozone column and haze.

A standard RATES file is provides with REMSAD. The heights above sea level at which the photolysis rates specified are fixed at 0, 150, 360, 640, 980, 1380, 1840, 2350, 2910, 3530, 4210, 6000, 8000, 10000, 12000, and 14000 m. The zenith angles for which the photolysis rates are specified are also fixed at 0, 10, 20, 30, 40, 50, 60, 70, 78, and 86 degrees. The constant value for albedo is 0.08, for ozone column is 0.318, and for haze is 0.2.

A standard RATES file for REMSAD, version 7 with micro-CB chemistry is provided in Exhibit 4-16.

4.6. Simulation Control Parameters

The instructions for carrying out the REMSAD simulation are contained in a control file. These include various simulation options, integration parameters, output specifications, and other parameters required by the REMSAD program.

The SIMCONTROL file contains the path names of all input/output files, initialization and termination times for the simulations, options for the simulation and data items that are not specified in other data files. Exhibit 4-17 lists and describes the input variables contained in this file, for each line or record of the SIMCONTROL file. Not all simulation parameters are required for all applications. In the exhibit, lines that may be left out of the control file under certain conditions are shaded. The conditions that allow the lines to be omitted are outlined in the description. Each line or record in the SIMCONTROL file has a specific format (which is also given in the table). Certain data values or data file names may not be used by REMSAD for some set of options but space for these items must still be allocated on the input line. These items are underlined, and the condition that requires that they have valid information is given in the description.

The control file input lines can be grouped into three categories: (1) input and output file unit numbers and filenames; (2) simulation run time information; and (3) modeling domain grid definition. Exhibit 4-18 contains an annotated, example control file.

4.6.1. Input and Output File Information

Input and output file unit numbers and filenames lines all have the same structure and contain two variables, the I/O file unit number and the file name, in that order. For those input and output files that are optional, the I/O file unit number also functions as a flag. File unit numbers greater than zero activate the option.

To restart a REMSAD simulation (using a previously generated output file), filenames indicating the path to the coarse- and nested-grid restart (or instantaneous concentration) files are required. A restart is indicated by setting the LRSTRT flag to "TRUE". The default file units for restarting REMSAD are 98 and 99 for the coarse grid and all nested grids. respectively. If there are no nested grids, only the filename for the coarse grid concentration file is required. Note that the output and thus the restart information for all nested grids is contained in a single file.

4.6.1.1.   *Simulation Run Time Information*

Simulation run time information consists of a list of chemical species to be output, a series of logical flags to indicate the simulation setup and information on the simulation time span, update interval, output print interval and maximum time step for the advection calculation. The simulation flags are listed and described in Table 4-4.

Table 4-4.
REMSAD Simulation Flag Definitions

Flag	Definition
LRSTRT	if = .TRUE., this is a restart of a previous run and restart files are required to reinitialize the model. (See FNCONC and FNFCONC)
LDEPN	if = .TRUE. dry deposition calculations are made during the simulation.
LWET	if LWET = .TRUE. wet deposition calculations are made during the simulation. A rainfall rate data file is required.
LSED	if LSED =.TRUE., species-dependent settling velocities are calculated for particulate matter depositions.
LPMCHM	if = .TRUE. aerosol chemistry calculations are made during the simulation. Emission input file(s) are required.
LTXCHM	if = .TRUE. toxic chemistry calculations are made during the simulation. Emission input file(s) are required.
LCART	= .TRUE., when Cartesian coordinates are used (km);
	= .TRUE. with UTMZONE=0, when Lambert conformal coordinates are used (km).
	= .FALSE., when lat/long coordinates (in degrees) are used.
LAREA	if = .TRUE., area source emissions are included in simulation.
LPTS	if = .TRUE., elevated point sources are included in simulation.
L1EDAY	if = .TRUE., only the time on the EMISSIONS file is required to match the modeled time, but date is not checked, thus the same file can be used for multiple simulation days.
	if = .FALSE., both date and time are required to match modeled date and time.
L1DAY	if = .TRUE., only the time on the meteorological data files is required to match modeled time; the date is not checked. Thus the same data files can be used for multiple days of simulation.
	if = .FALSE., both date and time on files are required to match modeled date and time.
LSTAGR	if = .TRUE., horizontal wind components on input data file(s) are defined at cell interfaces as in an Arakawa-C grid.
	if = .FALSE., horizontal wind components are defined at cell centers.
LMECH	if = .TRUE., mikcro CB-IV chemical mechanisms is invoked.
	if = .FALSE., parameterized chemistry is used.
LO3	if = .TRUE., need ozone and OH file (LMON and LMECH must be FALSE)
	if = .FALSE., do not need ozone and OH file

The species should correspond to those being simulated. Those given in the example SIMCONTROL file are typical for a simulation focusing on PM.

A line of text may be provided to document the simulation. This text is included in the output files and is used for file identification and tracking.

4.6.2.   Domain and Nested Grid Definition

The full modeling domain (coarse grid) and any nested grids are specified in the SIMCONTROL file. REMSAD supports the use of a Universal Transverse Mercator (UTM), latitude and longitude, or Lambert conformal coordinate system. The variable LCART is set to "TRUE" for Cartesian coordinates (units are kilometers) and to "FALSE" for latitude/longitude coordinates (units are degrees). The variable LCART is set to "TRUE" with UTMZONE equal to zero for the Lambert conformal coordinates (units are kilometers). The Lambert conformal option is a new feature. Most regional applications of REMSAD have used a latitude/longitude coordinate system.

4.6.2.1.   Vertical Structure

The vertical structure for each grid, coarse and nested, is designated by the σ value for the top of each layer. The σ values are listed in the SIMCONTROL file, as shown in Exhibit 4-18. In defining the vertical structure, the user must observe three rules:

1. The σ value for the surface must be equal to 1.

2. The σ value at the top of the modeling domain must be equal to 0.

3. Each σ level of the coarse grid must coincide with a σ level of all nested grids.

4.6.2.2.   Horizontal Nesting

The origin, dimensions, and resolution (in the x- and y-directions) of the coarse grid are specified in the SIMCONTROL file, as detailed in Exhibit 4-18.

The number of nested grids and the dimensions, starting point with the coarse grid, and ratio of coarse- to nested-grid resolution are also specified for each nested grid. All nested grids are defined relative to the coarse grid, even if they are nested within other nested grids. Nested-grid domains may be defined anywhere within the coarse grid, with some restrictions.

*   Nested-grid regions must be rectangles and must use the same number of subdivisions throughout a given nested grid; that is, no cell aggregation is allowed on the fine grids.

*   Nested grids may share a boundary, but cannot overlap.

*   For each consecutive level of nesting, the ratio of the resolution of the next outer grid to that for the nested grid must be an integer. (For instance, if fine grid one is nested within the coarse grid at a ratio of 3 to 1, and fine grid two is nested within fine grid one, the ratio of fine grid two to the coarse grid resolution could not be 5 to 1. The ratio of fine grid two to fine grid one would have to be 2 to 1 or greater so that the ratio of fine grid two to the coarse grid would be 6 to 1 or greater.)

*   The lower left corner of the nested grid cell (2,2) must align with the lower left corner of a coarse grid cell.

For each dimension of a nested grid, the number of cells is equal to the number of coarse-grid cells covered by the nested grid (the number of coarse-grid cells to be subdivided), multiplied by ratio of the coarse-grid-cell size to that for the nested grid, plus two. Two cells are added to each dimension for use by the advection scheme. Concentrations are not calculated for these boundary cells, but space is allocated for them in memory by the model. Input files must include

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values for these cells. Nested-grid output files contain values for these boundary cells, but they should not be used in any analyses.

Fine grids are numbered by the model as they are encountered during the definition process. The user must order the grid definitions such that outer grids are defined prior to inner grids.

Exhibit 4-1.
Structure of EMISSIONS file

Header Records
(1) The *File Description Header Record* contains 76 words:
1−10   A   File name = 'EMISSIONS '; 10 characters, one character per word.
11−70   A   File identifier; 60 characters, one character per word.
71   I   Number of segments; must be 1.
72   I   Number of chemical species.
The next four words describe the total time span contained on the file:
73   I   Beginning date of the file (Julian).
74   R   Beginning time of the file (hours).
75   I   Ending date of the file (Julian).
76   R   Ending time of the file (hours).
(2) The *Region Description Header Record* contains 15 words. The first three define the reference origin:
1   R   x-coordinate (UTM units).
2   R   y-coordinate (UTM units).
3   1   UTM zone.
The next two words define the location of the modeling region with respect to the reference origin:
4   R   x-location (meters).
5   R   y-location (meters).
The next two words define the size of each grid cell in the x- and y-directions:
6   R   Grid cell size, x-direction (meters).
7   R   Grid cell size, y-direction (meters).
The next three words define the size of the modeling region in grid cells:
8   I   Number of grid cells, x-direction.
9   I   Number of grid cells, y-direction.
10   I   Number of grid cells, z-direction.
The last five words describe the vertical distribution of grid cells. These values are not used in UAM-V.
11   I   Number of cells between surface layer and diffusion break.
12   I   Number of cells between diffusion break and top of region.
13   R   Height of surface layer (meters).
14   R   Minimum height of cells between surface layer and diffusion break (meters).
15   R   Minimum height of cells between diffusion break and top of region (meters).
(3) The *Segment Description Header Record* contains one group of four words for each segment (the number of segments appears in the File Description Header Record):
1   I   x-location of segment origin with respect to origin of modeling region (grid units).
2   I   y-location of segment origin with respect to origin of modeling region (grid units).
3   I   Number of grid cells in segment, x-direction.
4   I   Number of grid cells in segment, y-direction.
(4) The *Species Description Header Record* contains 10 words for each species (the number of species is defined in the File Description Header Record):
1−10   A   Species name; 10 characters, one character per word.

Time-Invariant Data
The EMISSIONS file contains no time-invariant data.

Time-Varying Data
The EMISSIONS file contains one set of the following two records for each time interval.
(1) The *Time Interval Record* contains four words:
1   I   Beginning date (Julian).
2   R   Beginning time (hours).
3   I   Ending date (Julian).
4   R   Ending time (hours).
(2) For the one segment of the region there is one *Emissions Record* for each species. The first 11 words of the record identify segment and species:
1   I   Segment number (must be 1).
2−11   A   Species name; 10 characters, one character per word.
The next series of words is the emissions array itself:
12+   R   Ground-level emissions (gram-moles per hour, or grams per hour for aerosols).

Exhibit 4-2.
Structure of PTSOURCE file

Header Records

(1) The *File Description Header Record* contains 76 words:

1-10	A	File name = 'PTSOURCE '; 10 characters, one character per word.
11-70	A	File identifier; 60 characters, one character per word.
71	I	Number of segments; must be 1.
72	I	Number of chemical species.

The next four words describe the total time span contained on the file.

73	I	Beginning date of the file (Julian).
74	R	Beginning time of the file (hours).
75	I	Ending date of the file (Julian).
76	R	Ending time of the file (hours).

(2) The *Region Description Header Record* contains 15 words. The first three define the reference origin:

1	R	x-coordinate (UTM units).
2	R	y-coordinate (UTM units).
3	I	UTM zone.

The next two words define the location of the modeling region with respect to the reference origin:

4	R	x-location (meters).
5	R	y-location (meters).

The next two words define the size of each grid cell in the x- and y-directions:

6	R	Grid cell size, x-direction (meters).
7	R	Grid cell size, y-direction (meters).

The next three words define the size of the modeling region in grid cells:

8	I	Number of grid cells, x-direction.
9	U	Number of grid cells, y-direction.
10	I	Number of grid cells, z-direction.

The last five words describe the vertical distribution of grid cells (not used in UAM-V):

11	I	Number of cells between surface layer and diffusion break.
12	I	Number of cells between diffusion break and top of region.
13	R	Height of surface layer (meters).
14	R	Minimum height of cells between surface layer and diffusion break (meters).
15	R	Minimum height of cells between diffusion break and top of region (meters).

(3) The *Segment Description Header Record* contains one group of four words for each segment (the number of segments appears in the File Description Header Record):

1	I	x-location of segment origin with respect to origin of modeling region (grid units).
2	I	y-location of segment origin with respect to origin of modeling region (grid units).
3	I	Number of grid cells in segment, x-direction.
4	I	Number of grid cells in segment, y-direction.

(4) The *Species Description Header Record* contains 10 words for each species (the number of species is defined in the File Description Header Record):

1-10	A	Species name; 10 characters, one character per word.

Time-Invariant Data

The PTSOURCE file contains the location and other fixed properties of each point source. For the one segment there are two records.

(1) The *Counter Record* contains two words:

1	I	Segment number (must be 1).
2	I	Number of point sources in segment.

(2) The *Point Source Definition Record* contains the following group of six words for each point source in the segment. If there are no point sources in the segment, this record does not appear:

1	R	x-coordinate of point source with respect to reference origin (meters).
2	R	y-coordinate of point source with respect to reference origin (meters).
3	R	Stack height (meters).
4	R	Stack diameter (meters).
5	R	Stack temperature (kelvins).
6	R	Stack exit velocity (meter/hour).

Time-Varying Data

The PTSOURCE file contains one set of the following records for each time interval.

(1) The *Time Interval Record* contains four words:

1	I	Beginning date (Julian).
2	R	Beginning time (hours).
3	I	Ending date (Julian).
4	R	Ending time (hours).

(2) There is a Counter Record, Point Source Location Record, and Point Source Emissions Record for each species in the one segment. The *Counter Record* contains two words:

1	I	Segment number (must be 1).
2	I	Number of point sources in the segment for this time interval. If the number of point sources defined in the Counter Record for time-invariant data is greater than zero, this number must also be greater than zero.

The *Point Source Location Record* contains the following group of five words for each point source in the segment. If there are no point sources in the segment, this record does not appear:

1	I	x-index within segment of cell to receive emissions.
2	I	y-index within segment of cell to receive emissions.
3	I	z-index of cell to receive emissions.
4	R	Flow rate (m^3/h).
5	R	Effective plume height (meters).

The *Point Source Emissions Record* contains the following group of words:

1	I	Segment number.
2-11	A	Species name; 10 characters, one character per word.
12+	R	Emissions (gram-moles per hour, or grams per hour for aerosols) from each point source.

Exhibit 4-3a.
Structure of the AIRQUALITY file

Header Records

(1) The *File Description Header Record* contains 76 words:

1–10	A	File name = 'AIRQUALITY'; 10 characters, one character per word.
11–70	A	File identifier; 60 characters, one character per word.
71	I	Number of segments; must be 1.
72	I	Number of chemical species.

The next four words describe the total time span contained on the file:

73	I	Beginning date of the file (Julian).
74	R	Beginning time of the file (hours).
75	I	Ending date of the file (Julian).
76	R	Ending time of the file (hours).

(2) The *Region Description Header Record* contains 15 words. The first three define the reference origin:

1	R	x-coordinate (UTM units).
2	R	y-coordinate (UTM units).
3	I	UTM zone.

The next two words define the location of the modeling region with respect to the reference origin:

4	R	x-location (meters).
5	R	y-location (meters).

The next two words define the size of each grid cell in the x- and y-directions:

6	R	Grid cell size, x-direction (meters).
7	R	Grid cell size, y-direction (meters).

The next three words define the size of the modeling region in grid cells (not used in UAM-V):

8	I	Number of grid cells, x-direction.
9	I	Number of grid cells, y-direction.
10	I	Number of grid cells, z-direction.

The last five words describe the vertical distribution of grid cells:

11	I	Number of cells between surface layer and diffusion break.
12	I	Number of cells between diffusion break and top of region.
13	I	Height of surface layer (meters).
14	R	Minimum height of cells between surface layer and diffusion break (meters).
15	R	Minimum height of cells between diffusion break and top of region (meters).

(3) The *Segment Description Header Record* contains one group of four words for each segment (number of segments appears in File Description Header Record; for CB-IV version of UAM, one segment is allowed):

1	I	x-location of segment origin with respect to origin of modeling region (grid units).
2	I	y-location of segment origin with respect to origin of modeling region (grid units).
3	I	Number of grid cells in segment, x-direction.
4	I	Number of grid cells in segment, y-direction.

(4) The *Species Description Header Record* contains 10 words for each species (the number of species is defined in the File Description Header Record):

Time-Invariant Data

The AIRQUALITY file contains no time-invariant data.

Time-Varying Data

The AIRQUALITY file contains one set of the following records for each time interval.

(1) The *Time Interval Record* contains four words:

1	I	Beginning date (Julian).
2	R	Beginning time (hours).
3	I	Ending date (Julian).
4	R	Ending time (hours).

(2) For the one segment of the region the AIRQUALITY file contains a set of *Concentration Records* for each species, ordered within each species by vertical level. First 11 words of record identify segment and species:

1	I	Segment number (must be 1).
2–11	A	Species name; 10 characters, one character per word.

The next series of words is the concentration array itself.

12+	R	Concentrations, units are ppm, except μg/(mole air) for SOA, POA, PEC, PMFINE, and

PMCOARS, for each cell in one vertical level, varying by x-, then y-direction.

Exhibit 4-3b.
Example AIRQUALITY Input File for a 140 by 104-Cell Domain with 15 Vertical Layers.

```
CONTROL
AIRQUALITY
INITIAL CONDITIONS Clean background
25          0          0          1          200        0
20          1          0
0           0          1          0          0          0
0           0          1          1          0          0
0           0          0          0          0          0
NO
NO2
O3
PAN
CO
HNO2
H2O2
HNO3
ISOP
CARB
VOC
NTR
SO2
SULF
NH3
PNO3
GSO4
ASO4
NH4N
NH4S
POA
PEC
SOA
PMFINE
PMCOARS
98001      0100       98365      2400
END
REGION
0.         0.              0
-138.0     20.1111
0.55556    0.37037
140        104        15
0          0          0.         0.         0.
END
UNITS
NO         PPB
NO2        PPB
O3         PPB
PAN        PPB
CO         PPB
HNO2       PPB
H2O2       PPB
HNO3       PPB
ISOP       PPB
CARB       PPB
```

```
VOC        PPB
NTR        PPB
SO2        PPB
SULF       PPB
NH3        PPB
PNO3       PPB
GSO4       PPB
ASO4       PPB
NH4N       PPB
NH4S       PPB
END
TIME INTERVAL
98001     0100      98365     2400
SUBREGION
A                   1         1         -1
END
METHOD
ALL       ALL       CONSTANT  0.        100000.   0
END
VERTICAL METHOD
ALL       ALL       CONSTANT  0.        100000.
END
CONSTANTS
ALL       NO        0.00000001
ALL       NO2       0.01000000
ALL       O3        34.0000000
ALL       PAN       0.01000000
ALL       CO        99.0000000
ALL       HNO2      0.00072880
ALL       H2O2      0.50000000
ALL       HNO3      0.50000000
ALL       ISOP      0.00000000
ALL       CARB      0.00010000
ALL       VOC       0.00010000
ALL       NTR       0.00010000
ALL       SO2       0.00010000
ALL       SULF      0.00010000
ALL       NH3       0.00010000
ALL       PNO3      0.00010000
ALL       GSO4      0.00010000
ALL       ASO4      0.00010000
ALL       NH4N      0.00010000
ALL       NH4S      0.00010000
ALL       POA       0.00000010
ALL       PEC       0.00000010
ALL       SOA       0.000000100
ALL       PMFINE    0.000000100
ALL       PMCOARS   0.000000100
END
ENDTIME
```

Exhibit 4-4a.
Structure of the BOUNDARY file

Header Records

(1) The *File Description Header Record* contains 76 words.

1−10	A	File name = 'BOUNDARY '; 10 characters, one character per word.
11−70	A	File identifier; 60 characters, one character per word.
71	I	Number of segments; must be 1.
72	I	Number of chemical species.

The next four words describe the total time span contained on the file:

73	I	Beginning date of the file (Julian).
74	R	Beginning time of the file (hours).
75	I	Ending date of the file (Julian).
76	R	Ending time of the file (hours).

(2) The *Region Description Header Record* contains 15 words. The first three define the reference origin:

1	R	x-coordinate (UTM units).
2	R	y-coordinate (UTM units).
3	I	UTM zone.

The next two words define the location of the modeling region with respect to the reference origin:

4	R	x-location (meters).
5	R	y-location (meters).

The next two words define the size of each grid cell in the x- and y-directions:

6	R	Grid cell size, x-direction (meters).
7	R	Grid cell size, y-direction (meters).

The next three words define the size of the modeling region in grid cells:

8	I	Number of grid cells, x-direction.
9	I	Number of grid cells, y-direction.
10	I	Number of grid cells, z-direction.

The last five words describe the vertical distribution of grid cells (not used in UAM-V):

11	I	Number of cells between surface layer and diffusion break.
12	I	Number of cells between diffusion break and top of region.
13	R	Height of surface layer (meters).
14	R	Minimum height of cells between surface layer and diffusion break (meters).
15	R	Minimum height of cells between diffusion breaks and top of region (meters).

(3) The *Segment Description Header Record* contains one group of four words for the one segment (number of segments must be 1 in the File Description Header Record):

1	I	x-location of segment origin with respect to origin of modeling region (grid units).
2	I	y-location of segment origin with respect to origin of modeling region (grid units).
3	I	Number of grid cells in segment, x-direction.
4	I	Number of grid cells in segment, y-direction.

(4) The *Species Description Header Record* contains 10 words for each species (number of species is defined in the File Description Header Record):

1−10	A	Species name; 10 characters, one character per word.

Time-Invariant Data

The BOUNDARY file defines the boundaries of the region, both the external boundaries defined in the data preparation and the internal segment interfaces created when the region is segmented.

For each segment there are four *Boundary Definition Records*, one record for each edge. The edges are defined as follows:

1	Left	West	lower limit column index for each row
2	Right	East	upper limit column index for each row
3	Bottom	South	lower limit row index for each column
4	Top	North	upper limit row index for each column

Each Boundary Definition Record defines the location of the boundary cells at an edge of a segment. The first three words identify the edge and its dimensions:

1	I	Segment number (must be 1).
2	I	Edge number.
3	I	Number of cells on edge (i.e., number of rows or columns).

The next four words define the boundary location for the grid index (row or column) along each edge:

4	I	Index, within the segment, of the cell at the edge of the region modeled (i.e., the first or last cell simulated within the row or column). If this number if 0, this row or column is omitted from the simulation and the next three numbers are ignored.
5	I	Segment number in which adjacent cell is located. If this number is 0, the boundary is an external one, and the next two numbers are ignored.
6	I	x-index of adjacent cell within segment defined in word 5.
7	I	y-index of adjacent cell within segment defined in word 5.

Time-Varying Data

The BOUNDARY file contains one set of the following records for each time interval.

 (1) The *Time Interval Record* contains four words:

1	I	Beginning date (Julian).
2	R	Beginning time (hours).
3	I	Ending date (Julian).
4	R	Ending time (hours).

(2) For each segment of the region, there is a set of *Boundary Concentration Records*, grouped by species, with four records (one for each edge) for each species. The first 12 words of the record identify the segment, species, and edge:

1	I	Segment number (must be 1).
2–11	A	Species name: 10 characters, one character per word.
12	I	Edge number.

The next series of words is the boundary concentration array on the vertical plane along the edge:

13+	R	Boundary concentrations, units are ppm, except μg/(mole air) for SOA, POA, PEC, PMFINE, and
		PMCOARS, at each vertical level for each cell along the edge. For rows or columns that are not to be simulated and for edges that represent internal segment boundaries, these numbers must be present but are ignored.

Exhibit 4-4b.
Example BOUNDARY Input File for a 140 by 104-Cell Domain with 15 Vertical Layers.

```
CONTROL
BOUNDARY
Clean boundaries everywhere
25         0          4          0          0          0
20         1          0          0          0          0
0          0          1          0          0          0
0          0          1          0          0          0
0          0          0          0          0          0
NO
NO2
O3
PAN
CO
HNO2
H2O2
HNO3
ISOP
CARB
VOC
NTR
SO2
SULF
NH3
PNO3
GSO4
ASO4
NH4N
NH4S
POA
PEC
SOA
PMFINE
PMCOARS
98001     0100       98365      2400
END
REGION
0.         0.             0
-138.0     20.11111
0.55556    0.37037
140        104        15
0          0          0.         0.         0.
END
UNITS
NO         PPB
NO2        PPB
O3         PPB
PAN        PPB
CO         PPB
HNO2       PPB
H2O2       PPB
HNO3       PPB
ISOP       PPB
CARB       PPB
```

```
VOC        PPB
NTR        PPB
SO2        PPB
SULF       PPB
NH3        PPB
PNO3       PPB
GSO4       PPB
ASO4       PPB
NH4N       PPB
NH4S       PPB
END
BOUNDARIES
SOUTH    -126.0549 20.7      -69.3333  20.7
EAST1    -69.3333  20.7      -61.0     54.0259
NORTH1   -137.166  54.0259   -61.0     54.0259
WEST1    -126.0549 20.7      -137.166  54.0259
END
TIME INTERVAL
     98001     0100     98365     2400
METHOD
ALL      ALL      BOUNDVALUE 0.0     100000.
END
VERTICAL METHOD
ALL      ALL      CONSTANT  0.000     100000.
END
BOUNDARYREADINGS
ALL      NO       0.00000001
ALL      NO2      0.01000000
ALL      O3       34.0000000
ALL      PAN      0.01000000
ALL      CO       99.0000000
ALL      HNO2     0.00115800
ALL      H2O2     0.50000000
ALL      HNO3     0.50000000
ALL      ISOP     0.00000000
ALL      CARB     0.00010000
ALL      VOC      0.00010000
ALL      NTR      0.00010000
ALL      SO2      0.00010000
ALL      SULF     0.00010000
ALL      NH3      0.00010000
ALL      PNO3     0.00010000
ALL      GSO4     0.00010000
ALL      ASO4     0.00010000
ALL      NH4N     0.00010000
ALL      NH4S     0.00010000
ALL      POA      0.00000100
ALL      PEC      0.00000100
ALL      SOA      0.00000100
ALL      PMFINE   0.00000100
ALL      PMCOARS  0.00000100
END
ENDTIME
```

Exhibit 4-5.
Wind fields file format (WIND)

Word	Type	Description
Record 1		
1	R	Beginning time (hour) of data interval
	I	Beginning date (format: yymmdd or yyjjj) of data interval
Record 2		
1+	R	U horizontal wind component for each cell, varying by x-, then y-directions for each layer
Record 3		
1+	R	V horizontal wind component for each cell, varying by x-, then y-directions for each layer

Exhibit 4-6.
Temperature file format (TEMPERATURE)

Word	Type	Description
Record 1		
1	R	Beginning time (hour) of data interval
2	I	Beginning date (format: yymmdd or yyjjj) of data interval
3+	R	Surface temperature (deg K) varying by x-, then y-directions.
Record 2		
1	R	Beginning time (hour) of data interval
2	I	Beginning date (format: yymmdd or yyjjj) of data interval
3+	R	Air temperature (deg K) varying by x-, then y-directions (record 2 is repeated for each layer)

Exhibit 4-7.
Surface pressure file format (PSURF)

Word	Type	Description
1	R	Beginning time (hour) of data interval
2	I	Beginning date (format: yymmdd or yyjjj) of data interval
3+	R	Surface pressure (mb) varying by x-, then y-directions.

Exhibit 4-8.
Water vapor concentration file format (H2O).

Word	Type	Description
1	R	Beginning time (hour) of data interval
2	I	Beginning date (format: yymmdd or yyjjj) of data interval
3+	R	Water vapor concentration (kg/kg) varying by x-, then y-directions (record is repeated for each layer).

Exhibit 4-9.
Vertical turbulent exchange coefficients Kv (diffusion).

Word	Type	Description
1	R	Beginning time (hour) of data interval
2	I	Beginning date (format: yymmdd or yyjjj) of data interval
3+	R	K_v (m^2/sec) for each cell, varying by x-, then y-directions (record is repeated for each layer).

Exhibit 4-10.
Cloud Liquid Water Mixing Ratio file format (CLW).

Word	Type	Description
1	R	Beginning time (hour) of data interval
2	I	Beginning date (format: yymmdd or yyjjj) of data interval
3+	R	Cloud liquid water concentration (kg/kg) varying by x-, then y-directions (record is repeated for each layer).

Exhibit 4-11.
Rain Liquid Water Mixing Ratio file format (RLW).

Word	Type	Description
1	R	Beginning time (hour) of data interval
2	I	Beginning date (format: yymmdd or yyjjj) of data interval
3+	R	Rain liquid water concentration (kg/kg) varying by x-, then y-directions (record is repeated for each layer).

Exhibit 4-12.
Precipitation rate file format (RAIN).

Word	Type	Description
1	R	Beginning time (hour) of data interval
2	I	Beginning date (format: yymmdd or yyjjj) of data interval
3+	R	Rainfall (inches/hr) for each cell, varying by x-, then y-directions.

Exhibit 4-13.
Surface characteristics file format (SURFACE).

Word	Type	Description
1+	R	Fraction of land-use category for each cell, varying by x-, then y-directions for each land-use type.

Exhibit 4-14.
Terrain height file format (TERRAIN).

Record 1		
Word	*Type*	*Description*
1+	R	Average height of surface above sea level (m) for each cell, varying by x-, then y-directions.

Exhibit 4-15.
Chemistry parameter file format (CHEMPARAM)

Line	*Contents*	*Format*	*Option Flags*
1	FTYPE	A	File type, must be CHEMPARAM
2	NID	A	File identifier, comment text
3	NSPECS	10X,I2	Number of species to be simulated; must equal number of species specified in control file.
4	NSIZE	10X,I2	Number of particle size distributions
5	NSPEC1	10X,I2	Number of micro-cb species (include if lmech = .true.)
6	NREACT	10X,I2	Number of micro-cb reactions (include if lmech = .true.)
7	STRNG	A	Descriptive text ignored by the program
8	AFDEF	F10.0	Default aromatic fraction (f_A, recommended value = 0.33)
9	STRNG	A	Descriptive text ignored by the program
10	PSIZE	8F7.3	Particle size (microns)
11	STRNG	A	Descriptive text ignored by the program
12[+]	MDIST	8F7.3	Mass distributions for each designated particle size
13	STRNG	A	Descriptive text ignored by the program
14[+]	MSNO	I2	Simulated species number
	EFLAG	X,A1	
	MSPEC	X,10A1	Names of species to be simulated, must match names in the control file
	SZDIST	F10.2	Particle size flag, index to size distribution
	RHOP	F10.2	Particle density (g/cm^3)
	FC	E10.2	Hygroscopic affinity factor
	BDNL		Boundary layer concentration

Exhibit 4-16.
Standard photolysis rates file with micor-CB chemistry (RATES).

O3 Column =0.318 Albedo =0.080 Haze O.D. =0.200
0.000 = Current altitude in km

5.142E-01	5.089E-01	4.926E-01	4.646E-01	4.235E-01	3.668E-01	2.908E-01	1.913E-01	9.841E-02	2.578E-02
1.783E-03	1.750E-03	1.652E-03	1.489E-03	1.265E-03	9.857E-04	6.662E-04	3.410E-04	1.264E-04	1.635E-05
2.434E-03	2.400E-03	2.297E-03	2.124E-03	1.877E-03	1.550E-03	1.142E-03	6.688E-04	2.954E-04	5.311E-05
1.964E-03	1.891E-03	1.681E-03	1.362E-03	9.810E-04	5.969E-04	2.772E-04	7.931E-05	1.557E-05	1.104E-06
3.180E-04	3.097E-04	2.855E-04	2.470E-04	1.969E-04	1.400E-04	8.264E-05	3.445E-05	9.944E-06	8.797E-07

0.150 = Current altitude in km

5.522E-01	5.469E-01	5.306E-01	5.025E-01	4.611E-01	4.037E-01	3.255E-01	2.208E-01	1.190E-01	3.405E-02
1.951E-03	1.917E-03	1.815E-03	1.645E-03	1.411E-03	1.116E-03	7.732E-04	4.143E-04	1.654E-04	2.552E-05
2.662E-03	2.627E-03	2.522E-03	2.344E-03	2.088E-03	1.748E-03	1.315E-03	7.990E-04	3.727E-04	7.547E-05
2.150E-03	2.072E-03	1.848E-03	1.506E-03	1.095E-03	6.774E-04	3.245E-04	9.999E-05	2.318E-05	2.376E-06
3.477E-04	3.390E-04	3.135E-04	2.728E-04	2.197E-04	1.586E-04	9.634E-05	4.256E-05	1.371E-05	1.620E-06

0.360 = Current altitude in km

5.746E-01	5.693E-01	5.533E-01	5.257E-01	4.847E-01	4.275E-01	3.489E-01	2.414E-01	1.333E-01	3.908E-02
2.060E-03	2.025E-03	1.922E-03	1.749E-03	1.509E-03	1.205E-03	8.465E-04	4.642E-04	1.913E-04	3.163E-05
2.806E-03	2.771E-03	2.666E-03	2.487E-03	2.227E-03	1.880E-03	1.433E-03	8.876E-04	4.242E-04	9.022E-05
2.278E-03	2.197E-03	1.963E-03	1.607E-03	1.176E-03	7.348E-04	3.581E-04	1.142E-04	2.817E-05	3.211E-06
3.675E-04	3.585E-04	3.323E-04	2.903E-04	2.353E-04	1.716E-04	1.059E-04	4.810E-05	1.620E-05	2.109E-06

0.640 = Current altitude in km

5.954E-01	5.903E-01	5.746E-01	5.476E-01	5.074E-01	4.508E-01	3.722E-01	2.625E-01	1.483E-01	4.398E-02
2.170E-03	2.135E-03	2.030E-03	1.855E-03	1.609E-03	1.296E-03	9.226E-04	5.163E-04	2.181E-04	3.790E-05
2.949E-03	2.914E-03	2.809E-03	2.628E-03	2.367E-03	2.013E-03	1.553E-03	9.797E-04	4.776E-04	1.052E-04
2.411E-03	2.326E-03	2.084E-03	1.713E-03	1.261E-03	7.959E-04	3.939E-04	1.292E-04	3.331E-05	4.067E-06
3.877E-04	3.786E-04	3.517E-04	3.084E-04	2.515E-04	1.851E-04	1.159E-04	5.391E-05	1.876E-05	2.609E-06

0.980 = Current altitude in km

6.150E-01	6.100E-01	5.947E-01	5.683E-01	5.289E-01	4.732E-01	3.950E-01	2.836E-01	1.637E-01	4.884E-02
2.281E-03	2.245E-03	2.139E-03	1.961E-03	1.711E-03	1.389E-03	1.001E-03	5.702E-04	2.459E-04	4.431E-05
3.089E-03	3.055E-03	2.949E-03	2.769E-03	2.506E-03	2.147E-03	1.675E-03	1.074E-03	5.330E-04	1.205E-04
2.548E-03	2.460E-03	2.208E-03	1.822E-03	1.350E-03	8.598E-04	4.317E-04	1.450E-04	3.857E-05	4.943E-06
4.084E-04	3.990E-04	3.714E-04	3.269E-04	2.681E-04	1.990E-04	1.262E-04	5.994E-05	2.141E-05	3.121E-06

1.380 = Current altitude in km

6.340E-01	6.291E-01	6.142E-01	5.885E-01	5.499E-01	4.951E-01	4.174E-01	3.048E-01	1.798E-01	5.386E-02
2.393E-03	2.357E-03	2.250E-03	2.069E-03	1.815E-03	1.484E-03	1.082E-03	6.266E-04	2.750E-04	5.095E-05
3.231E-03	3.196E-03	3.091E-03	2.911E-03	2.647E-03	2.284E-03	1.800E-03	1.173E-03	5.913E-04	1.362E-04
2.690E-03	2.600E-03	2.339E-03	1.937E-03	1.443E-03	9.273E-04	4.718E-04	1.617E-04	4.408E-05	5.854E-06
4.296E-04	4.200E-04	3.917E-04	3.459E-04	2.852E-04	2.135E-04	1.371E-04	6.630E-05	2.418E-05	3.651E-06

1.840 = Current altitude in km

6.528E-01	6.481E-01	6.336E-01	6.084E-01	5.707E-01	5.167E-01	4.397E-01	3.262E-01	1.965E-01	5.918E-02
2.507E-03	2.471E-03	2.363E-03	2.180E-03	1.921E-03	1.582E-03	1.165E-03	6.858E-04	3.058E-04	5.786E-05
3.373E-03	3.339E-03	3.234E-03	3.054E-03	2.789E-03	2.422E-03	1.928E-03	1.275E-03	6.532E-04	1.524E-04
2.840E-03	2.746E-03	2.475E-03	2.057E-03	1.542E-03	9.986E-04	5.145E-04	1.796E-04	4.985E-05	6.805E-06
4.515E-04	4.417E-04	4.126E-04	3.656E-04	3.030E-04	2.286E-04	1.484E-04	7.300E-05	2.710E-05	4.203E-06

2.350 = Current altitude in km

6.714E-01	6.668E-01	6.527E-01	6.281E-01	5.911E-01	5.381E-01	4.617E-01	3.475E-01	2.136E-01	6.478E-02
2.622E-03	2.585E-03	2.476E-03	2.291E-03	2.028E-03	1.681E-03	1.251E-03	7.467E-04	3.378E-04	6.488E-05
3.515E-03	3.481E-03	3.377E-03	3.197E-03	2.931E-03	2.562E-03	2.058E-03	1.380E-03	7.176E-04	1.690E-04
2.993E-03	2.896E-03	2.615E-03	2.181E-03	1.643E-03	1.073E-03	5.591E-04	1.983E-04	5.579E-05	7.773E-06
4.736E-04	4.635E-04	4.338E-04	3.856E-04	3.211E-04	2.439E-04	1.601E-04	7.995E-05	3.012E-05	4.765E-06

2.910 = Current altitude in km

6.901E-01	6.856E-01	6.718E-01	6.477E-01	6.115E-01	5.593E-01	4.836E-01	3.690E-01	2.313E-01	7.077E-02
2.736E-03	2.699E-03	2.589E-03	2.402E-03	2.135E-03	1.782E-03	1.337E-03	8.096E-04	3.712E-04	7.200E-05
3.656E-03	3.622E-03	3.519E-03	3.339E-03	3.073E-03	2.701E-03	2.189E-03	1.488E-03	7.852E-04	1.858E-04
3.150E-03	3.050E-03	2.759E-03	2.308E-03	1.748E-03	1.150E-03	6.059E-04	2.181E-04	6.193E-05	8.758E-06
4.958E-04	4.856E-04	4.552E-04	4.058E-04	3.395E-04	2.596E-04	1.721E-04	8.717E-05	3.326E-05	5.334E-06

3.530 = Current altitude in km

7.091E-01	7.047E-01	6.912E-01	6.677E-01	6.322E-01	5.810E-01	5.061E-01	3.912E-01	2.500E-01	7.737E-02
2.851E-03	2.814E-03	2.703E-03	2.515E-03	2.244E-03	1.884E-03	1.427E-03	8.758E-04	4.069E-04	7.936E-05
3.798E-03	3.764E-03	3.661E-03	3.483E-03	3.217E-03	2.843E-03	2.323E-03	1.601E-03	8.577E-04	2.034E-04
3.313E-03	3.210E-03	2.909E-03	2.441E-03	1.858E-03	1.231E-03	6.558E-04	2.393E-04	6.842E-05	9.771E-06
5.186E-04	5.081E-04	4.771E-04	4.265E-04	3.584E-04	2.759E-04	1.846E-04	9.481E-05	3.660E-05	5.920E-06

4.210 = Current altitude in km									
7.281E-01	7.238E-01	7.107E-01	6.878E-01	6.531E-01	6.029E-01	5.290E-01	4.143E-01	2.700E-01	8.479E-02
2.966E-03	2.929E-03	2.818E-03	2.628E-03	2.354E-03	1.989E-03	1.520E-03	9.454E-04	4.453E-04	8.700E-05
3.938E-03	3.904E-03	3.803E-03	3.626E-03	3.361E-03	2.986E-03	2.461E-03	1.719E-03	9.360E-04	2.219E-04
3.482E-03	3.374E-03	3.064E-03	2.579E-03	1.972E-03	1.317E-03	7.091E-04	2.623E-04	7.533E-05	1.081E-05
5.416E-04	5.310E-04	4.993E-04	4.477E-04	3.778E-04	2.927E-04	1.977E-04	1.029E-04	4.018E-05	6.524E-06
6.000 = Current altitude in km									
7.709E-01	7.669E-01	7.546E-01	7.332E-01	7.007E-01	6.532E-01	5.826E-01	4.700E-01	3.213E-01	1.067E-01
3.225E-03	3.188E-03	3.077E-03	2.886E-03	2.609E-03	2.234E-03	1.743E-03	1.121E-03	5.483E-04	1.068E-04
4.249E-03	4.217E-03	4.119E-03	3.947E-03	3.688E-03	3.317E-03	2.787E-03	2.013E-03	1.145E-03	2.725E-04
3.886E-03	3.771E-03	3.438E-03	2.915E-03	2.256E-03	1.532E-03	8.467E-04	3.236E-04	9.372E-05	1.337E-05
5.950E-04	5.840E-04	5.511E-04	4.972E-04	4.237E-04	3.332E-04	2.302E-04	1.238E-04	4.977E-05	8.038E-06
8.000 = Current altitude in km									
8.081E-01	8.044E-01	7.931E-01	7.733E-01	7.433E-01	6.992E-01	6.330E-01	5.255E-01	3.776E-01	1.378E-01
3.460E-03	3.424E-03	3.314E-03	3.125E-03	2.849E-03	2.471E-03	1.968E-03	1.311E-03	6.735E-04	1.329E-04
4.523E-03	4.492E-03	4.398E-03	4.234E-03	3.986E-03	3.626E-03	3.105E-03	2.320E-03	1.392E-03	3.441E-04
4.295E-03	4.174E-03	3.819E-03	3.262E-03	2.553E-03	1.765E-03	1.001E-03	3.970E-04	1.167E-04	1.621E-05
6.459E-04	6.346E-04	6.009E-04	5.453E-04	4.691E-04	3.742E-04	2.643E-04	1.473E-04	6.160E-05	9.872E-06
10.000 = Current altitude in km									
8.363E-01	8.329E-01	8.225E-01	8.042E-01	7.765E-01	7.358E-01	6.745E-01	5.738E-01	4.313E-01	1.770E-01
3.652E-03	3.617E-03	3.509E-03	3.325E-03	3.053E-03	2.678E-03	2.172E-03	1.496E-03	8.106E-04	1.693E-04
4.736E-03	4.707E-03	4.618E-03	4.463E-03	4.227E-03	3.883E-03	3.379E-03	2.604E-03	1.651E-03	4.462E-04
4.684E-03	4.557E-03	4.185E-03	3.597E-03	2.844E-03	1.998E-03	1.163E-03	4.789E-04	1.444E-04	1.944E-05
6.907E-04	6.792E-04	6.450E-04	5.883E-04	5.102E-04	4.122E-04	2.971E-04	1.714E-04	7.509E-05	1.224E-05
12.000 = Current altitude in km									
8.572E-01	8.541E-01	8.445E-01	8.277E-01	8.021E-01	7.646E-01	7.081E-01	6.149E-01	4.806E-01	2.234E-01
3.814E-03	3.780E-03	3.676E-03	3.496E-03	3.230E-03	2.861E-03	2.359E-03	1.675E-03	9.571E-04	2.218E-04
4.903E-03	4.876E-03	4.792E-03	4.645E-03	4.422E-03	4.096E-03	3.614E-03	2.863E-03	1.911E-03	5.883E-04
5.085E-03	4.952E-03	4.562E-03	3.945E-03	3.149E-03	2.246E-03	1.340E-03	5.736E-04	1.789E-04	2.354E-05
7.325E-04	7.209E-04	6.862E-04	6.288E-04	5.493E-04	4.488E-04	3.295E-04	1.964E-04	9.043E-05	1.561E-05
14.000 = Current altitude in km									
8.726E-01	8.697E-01	8.607E-01	8.451E-01	8.215E-01	7.869E-01	7.349E-01	6.490E-01	5.245E-01	2.743E-01
3.958E-03	3.925E-03	3.824E-03	3.650E-03	3.391E-03	3.029E-03	2.534E-03	1.849E-03	1.111E-03	2.943E-04
5.036E-03	5.011E-03	4.932E-03	4.793E-03	4.582E-03	4.273E-03	3.815E-03	3.095E-03	2.163E-03	7.715E-04
5.541E-03	5.402E-03	4.993E-03	4.342E-03	3.499E-03	2.533E-03	1.548E-03	6.899E-04	2.241E-04	2.930E-05
7.750E-04	7.633E-04	7.283E-04	6.701E-04	5.893E-04	4.865E-04	3.632E-04	2.233E-04	1.080E-04	2.047E-05

Exhibit 4-17.
Simulation Control File Contents and Format (SIMCONTROL)

Line	Contents	Format	Description and Option Flags
1	IOUT1	I2	= 66, Unit number of ATDM output information file (SIMOUT)
	FNOUT	A	Name of ATDM (formatted) output information file showing program control (SIMOUT)
2	IOUT2	I2	= 8, Unit number of ATDM diagnostic output file (DIAG)
	FNDIAG	A	Name of ATDM (formatted) diagnostic output file (DIAG)
3	IAVG	I2	Unit number of coarse-grid average concentration file
	FNAVG	A	Name of coarse-grid hourly first-layer average concentration file; opened only when IAVG > 0 else may be /dev/null
4[+]	NAVSPC	I2	Number of species to be output for average concentrations
	MAVSPC(*)	6A10,/, 2X, 6A10	Name of each species L to be output for average concentrations. Note that these same species are written to both the FNAVG (coarse-grid average) file and the FNFAVG (fine-grid average) file. (Species not in this list are not written to the average concentration files.) If the offline storage file for ozone, radicals, and other species is to be written during the simulation, the species name OH should be included as the last name in this list. Note that OH will not be written to the average concentration file, but will be included in the offline file.
5	IDEP	I2	Unit number of coarse-grid output deposition file
	FNDEP	A	File name of coarse-grid deposition file. opened only when IDEP > 0 else may be /dev/null
6	IINST	I2	= 51, Unit number of coarse-grid instantaneous concentration file
	FNINST	A	Name of coarse-grid instantaneous concentration file
7	IFAVG	I2	Unit number of fine-grid average concentration file
	FNFAVG	A	Name of fine-grid hourly 1st-layer average concentration file; opened only when IFAVG > 0 else may be /dev/null
8	IFDEP	I2	Nested grids' deposition output flag/file unit (IFDEP > 0)
	FNFDEP	A	Nested grids' Domain deposition output file name. opened only when IFDEP > 0 else may be /dev/null
9	IFINST	I2	Nested grids' instantaneous concentration output file unit
	FNFINST	A	Nested grids' instantaneous concentration file name, opened only when IFINST > 0 else may be /dev/null
10	MSG	A80	Message or ATDM run title
11	LRSTRT	L10	if = .TRUE., this is a restart of a previous run and restart files are required to reinitialize the model.
	LDEPN	L10	if = .TRUE. dry deposition calculations are made during the simulation
	LWET	L10	if LWET = .TRUE. wet deposition calculations are made during the simulation. A rainfall data file is required.
	LSED	L10	if LSED = .TRUE., species-dependent settling velocities are calculated for particulate matter depositions.
	LPMCHM	L10	if = .TRUE. , aerosol chemistry calculations are made and emission inputs are required
	LTXCHM	L10	if = .TRUE. , toxic chemistry calculations are made and emission inputs are required
	LMECH	L10	if = .TRUE. , micro CM-IV chemical mechanism is invoked; if = .FALSE., parameterized chemistry is used.

Line	Contents	Format	Description and Option Flags
12	LCART	L10	= .TRUE., when Cartesian coordinates are used (km); = .FALSE., when lat/long coordinates (in degrees) are used. = .TRUE. with UTMZONE=0 when Lambert Conformal coordinates are used (km)
	LAREA	L10	if = .TRUE., area source emissions are included in simulation
	LPTS	L10	if = .TRUE., point source emissions are included in simulation
	L1EDAY	L10	if = .TRUE., only the time on the EMISSIONS file is required to match the modeled time, but the date is not checked. Thus the same file can be used for multiple days of simulation. if = .FALSE., both date and time are required to match modeled date and time.
	L1DAY	L10	if = .TRUE., only the time on the meteorological data files is required to match modeled time; the date is not checked. Thus the same data files can be used for multiple days of simulation. if = .FALSE., both date and time on files are required to match modeled date and time
	LSTAGR	L10	if = .TRUE., horizontal wind components on input data file(s) are defined at cell interfaces as in an Arakawa-C grid. if = .FALSE., horizontal wind components are defined at cell centers
	LO3	L10	if = .TRUE., need ozone and OH file (LMON and LMECH must be FALSE) if = .FALSE., do not need ozone and OH file
13	TSTR	F10.0	Time at which the simulation is to begin; military hour, ex. 900.0 is 9 a.m)
	IDYSTR	I10	Date on which simulation is to begin, optionally calendar (YYMMDD) or Julian (YYJJJ) format; ex. February 3, 1990 is 900203 or 90034
	TEND	F10.0	Time at which simulation is to terminate.
	IDYNF	I10	Date on which simulation is to terminate (YYMMDD or YYJJJ)
	DTDATA	F10.0	Input meteorological data update interval, in military hour (i.e., 100. = 1 hour interval)
	DTPRNT	F10.0	Concentration output interval, in military hour
	DTSTEP	F10.0	Maximum time step for advection calculation, in minutes
14	DLONG	F10.0	East-west grid spacing, in degrees longitude if latitude/longitude coordinates are chosen; otherwise in km when Cartesian coordinates are used. (See LCART above.)
	DLAT	F10.0	North-south grid spacing, in degrees latitude or in km
	NOX	I10	Number of coarse-grid cells in the east-west direction
	NOY	I10	Number of coarse-grid cells in the north-south direction
	NLAYER	I10	Number of coarse-grid vertical layers
	NOSPEC	I10	Number of chemical species (must match the number on the CHEMPARAM file)
15	WLONG	F10.0	Longitude of west boundary of modeling region (negative value in western hemisphere), in degrees
	ELONG	F10.0	Longitude of east boundary of modeling region, in degrees
	SLAT	F10.0	Latitude of south boundary of modeling region, in degrees
	NLAT	F10.0	Latitude of north boundary of modeling region, in degrees
	TZ	F10.0	Time zone (5.0 = EST; 6.0 = CST; 7.0 = MST; 8.0 = PST; 0.0 = GMT)
	UTMZON	I10	UTM zone number of the modeling domain
16	XORG	F10.0	X coordinate of the origin (i.e. lower-left corner) of the modeling domain, in UTM km; it is a dummy variable if LCART = .FALSE.
	YORG	F10.0	Y coordinate of the origin of the modeling domain, in UTM km, it is a dummy variable if LCART = .FALSE.
17	PMODTOP	F6.3	Pressure at the tope of the modeling domain (mb)
	SIGMA(K), K=1,NLAYER)	20F6.3	σ pressure level at top of each layer
18	NUMFIN	I10	Number of fine ("nested") grids

Line	Contents	Format	Description and Option Flags
Read NUMFIN sets of the following block if NUMFIN > 0			
19[1]	IXFB	6I10	Lower left (SW) coarse grid cell covered by nested grid number IFINE.
	JYFB		
	IXFE		Upper right (NE) coarse grid cell covered by nested grid number IFINE.
	JYFE		
	NHF		Number of horizontal subdivisions along one dimension of coarse grid cells to match resolution of nested grid number IFINE. This is the ratio of the linear dimension of the cells (e.g., if NHF = 2, there are actually four fine grid cells per coarse grid cell).
	NFZ		Number of layers in fine grid number IFINE. If this value does not equal NLAYER, you must provide a HEIGHT/PRESSURE file for this fine grid. NZF may not be less than NLAYER.
20[1]	(SIGMAF(K), K=1,NFZ)	6X, 20F6.3	s pressure level at top of each layer
21	DTMIN	F10.0	Minimum allowable time step for chemistry integration, in hours. Recommended value is 0.00001
	MAXITR	I10	Minimum number of iterations for chemistry integration. Recommended value is 5
	RERROR	F10.0	Relative error tolerance for chemistry integration. Recommended value is 0.005
22	ICHEM	I2	Unit number of the chemistry parameter file
	FNCHEM	A	Name of (formatted) chemistry mechanism specification file, which includes species names, reaction rate constants, etc.
23	IHO1	I2	Unit number of the lower layer hydroxyl file
	FNOH1	A	Name of lower layer hydroxyl radical look-up table file
24	IOH2	I2	Unit number of the upper layer hydroxyl file
	FNOH2	A	Name of upper layer hydroxyl radical look-up table file
25	NPHVAL	I2	Unit number of photolysis rates file
	FNPH	A	Name of photolysis rates data file
26	IWIND	I2	Unit number of the coarse grid wind (WIND) file
	FNWIND	A	Name of the coarse grid WIND input file
27	IPRS	I2	Unit number of the coarse grid surface pressure (PSURF) file
	FNPRS	A	Name of the coarse grid surface pressure input file
28	ITEMP	I2	Unit number of temperature file (TEMPERATURE)
	FNTEMP	A	Name of temperature file
29	IH2O	I2	Unit number of water concentration file (H2O)
	FNH2O	A	Name of water vapor concentration file
30	ISURF	I2	Unit number of file containing surface-cover types (SURFACE)
	FNSURF	A	Name of surface-cover type file (SURFACE)
31	ITERR	I2	Unit number of terrain height data file (TERRAIN)
	FNTERR	A	Name of terrain height data file
32	IEDF	I2	Unit number of point source emissions file (PTSOURC)
	FNPNT	A	Name of point source emission file
33	IAEM1	I2	Unit number of the weekday low-level emission file (EMISSIONS)
	FNAEM1	A	Name of weekday low-level area source emission file
34	IAEM2	I2	Unit number of the Saturday low-level emission file (EMISSIONS)
	FNAEM2	A	Name of Saturday low-level source emission file, opened only when AEM2 > 0 else may be /dev/null
35	IAEM3	I2	Unit number of the Sunday low-level emission file (EMISSIONS)
	FNAEM3	A	Name of Sunday low-level source emission file, opened only when AEM3 > 0 else may be /dev/null
36	ICBC	I2	Unit number of initial concentration file (AIRQUALITY)
	FNIC	A	Name of initial concentration data file
37	IO3	I2	Unit number of the ozone concentration file (O3CONC)
	FNO3	A	Name of the ozone concentration file (the offline file saved from a prior run)

Line	Contents	Format	Description and Option Flags
38	IRAIN	I2	Unit number of rainfall data file (RAIN)
	FNRAIN	A	Name of rainfall data file (RAIN); must be present when LWET = .TRUE.
39	IKV	I2	Unit number of vertical diffusivity file (VDIFFUSION)
	FNKV	A	Name of vertical diffusivity file (VDIFFUSION)
40[1,2]	IFWIND	I2	Unit number of fine grid wind file (WIND)
	FNFWIND	A	Name of the fine grid wind file, opened only when NUMFIN > 0 and IFWIND > 0 (repeat line NUMFIN times).
41[1,2]	IFKV	I2	Unit number of vertical diffusivity data file for the *i*th fine grid domain
	FNFKV	A	Name of vertical diffusivity file for the *i*th fine grid domain; opened only when IFKV(I) > 0 (repeat line NUMFIN times).
42[1,2]	IFPRS	I2	Unit number of fine grid surface pressure file (PSURF)
	FNFPRS	A	Name of the fine grid wind file, opened only when NUMFIN > 0 and IFPRS > 0 (repeat line NUMFIN times).
43[1,2]	IFO3	I2	Unit number of fine grid ozone concentration file (O3CONC)
	FNFO3	A	Name of the fine grid ozone concentration file, the offline concentration file from a prior run, opened only when NUMFIN > 0 and IFO3 > 0 (repeat line NUMFIN times).
44[1,2]	IFSRF	I2	Unit number of fine grid surface file (SURFACE)
	FNFSRF	A	Name of the fine grid surface file, opened only when NUMFIN > 0 and IFSRF > 0 (repeat line NUMFIN times).
Read NUMFIN sets of the following block if NUMFIN > 0				
45[1]	IFAEM1	I2	Unit number of weekday area emission data file for the *i*th nested grid domain
	FNFAEM1	A	Name of weekday area emission data file for the *i*th nested grid domain.
46[1]	IFAEM2	I2	Unit number of Saturday area emission data file for the *i*th fine grid domain
	FNFAEM2	A	Name of Saturday area emission data file for the *i*th fine grid domain; opened only when IFAEM2(I) > 0 else may be /dev/null
47[1]	IFAEM3	I2	Unit number of Saturday area emission data file for the *i*th fine grid domain
	FNFAEM3	A	Name of Saturday area emission data file for the *i*th fine grid domain; opened only when IFAEM3 > 0 else may be /dev/null
48	ICBC	I2	Unit number of initial concentration file (AIRQUALITY)
	NBNDC	A	Name of the initial concentration file
49	IDEPV	I2	Unit number of deposition velocity file.
	FNDEPV	A	Name of the deposition velocity file, opened when IDEPV > 0 else may be /dev/null
50[1]	FNCONC (UNIT 98)	A	File name of coarse-grid instantaneous concentrations data file from the previous run, opened on unit number 98. Used for restarts.
51[1]	FNFCONC (UNIT 99)	A	File name of fine grid instantaneous concentrations data file from the previous run, opened on unit number 99. Used for restarts.

[1] Record *must* appear if the first option flag listed for this record is true, and *must not* appear if the flag is false
[2] Repeat this record NUMFIN times if NUMFIN > 0

Exhibit 4-18.
Annotated simulation control file (SIMCONTROL)

This run for criteria pollutants employs a single fine grid and produces an offline concentration file for use in later mercury simulations.

NOTE: when running the first simulation day, the restart flag (discussed below) should be set to `false`.
```
      ##############################################################
      #
      cat << -eof- > atdmin.0616.$scen[$j]
```

`out` *and* `diag` *files contain diagnostic information on the progress of the run.*
```
      66$OUTDIR/SYSO/atdm.0616.test.out
      08$OUTDIR/SYSO/atdm0616.test.diag
```

Coarse grid average file.
```
      67$OUTDIR/AVRG/atdm.0616.test.avrg
```

List of species to appear on the average files. NOTE: include `OH` *as the **last** species name in order to generate offline storage file for later mercury modeling.*
```
      37NO         NO2        NO2S       O3         CARB       VOC
         PAN       CO         HNO2       H2O2       HNO3       NTR
         SO2       SULF       ISOP       NH3        PNO3       GSO4
         ASO4      NH4N       NH4S       SOA        PEC        PMFINE
         PMCOARS   POA        PNA        TERP       SV1        SV2
         SV3       SV4        SOA1       SOA2       SOA3       SOA4
         OH
```

The coarse grid offline storage file contains radical and other species concentrations for use in later modeling. NOTE: this line is only included when `OH` *is specified as the last species above.*
```
      65$OFFDIR/off/atdm.0616.test.coarse
```

Coarse grid deposition file.
```
      69$OUTDIR/DEPN/atdm.0616.test.depn
```

Coarse grid instantaneous file.
```
      51$OUTDIR/INST/atdm.0616.test.inst
```

Fine grid average file.
```
      68$OUTDIR/AVRG/atdm.0616.test.favrg
```

Fine grid deposition file.
```
      70$OUTDIR/DEPN/atdm.0616.test.fdepn
```

Fine grid instantaneous file.
```
      52$OUTDIR/INST/atdm.0616.test.finst
```

The fine grid offline storage file contains radical and other species concentrations for use in later modeling. NOTE: this line is only included when `OH` *is specified as the last species above.*
```
      64$OFFDIR/off/atdm.0616.test.fine
```

Comment line, placed on header of average, deposition, and instantaneous files.
```
     ATDM PM Run: June 16, 1996 : Micro Mech Chemistry with ISOP&TERP
```

Simulation options -- see manual for further details. The first flag is the restart flag, set to true *when reinitializing from a prior simulation day.*
```
         true      true      true      true      true     false      true
        false      true      true      true     false     false     false
```

Start and end time and date, input and output intervals, and maximum time step. Please refer to manual.
```
        0000.0    960616    0000.0    960617     100.0     100.0      30.0
```

*Definition of the coarse grid domain. **D**x and **D**y (in appropriate units to match the grid system being used), number of x and y cells, number of layers, and number of species (must match number of species in chemparam file).*
```
        0.500     0.333       120        84        12        36
```

Extent of domain in longitude and latitude (starting and ending), and the time zone and UTM zone. UTM zone is set to -9 if using lati-long, and set to zero if using lambert conformal grid system.
```
       -126.00    -66.00     24.00     52.00        5.        -9
```

Origin of UTM or lambert conformal grid system, set to zero when using a latitude-longitude grid system.
```
         0.00      0.00
```

Pressure at top of domain, and sigma levels defining the model layers. Please see manual for further details.
```
       100. 0.9950 0.9880 0.9700 0.9380 0.8930 0.8390 0.7770 0.7020 0.5820
      0.4000 0.2000 0.0000
```

Number of nested (fine) grids.
```
     1
```

Starting x and y coarse grid cells for fine grid 1, ending x and y coarse grid cells for fine grid 1, ratio of horizontal fine to coarse cells, number of layers in the fine grid (must be >= number of layers in coarse grid). This line is written in 6i10 format.
```
          45        38       108        78         3        12
```

Sigma levels for fine grid 1.
```
           0.9950 0.9880 0.9700 0.9380 0.8930 0.8390 0.7770 0.7020 0.5820
      0.4000 0.2000 0.0000
```

Minimum time step, maximum number of iterations, and the error tolerance for gas-phase chemistry. NOTE: should be edited by advanced users only.
```
     1.00e-05         5     0.005
```

Unit numbers: the first two characters of the following lines can be any integer that is not used to define any other file. 00 *indicates the file will not be read by the model. The units used for model output files (*66, 08, 67, 65, 69, 51, 68, 70, 52, *and* 64*) should not be altered, nor should they be used below.*

Chemparam file containing list of species to be simulated, and gas phase chemistry reaction rates. Supplied with the model. NOTE: ordinarily should not be altered by the user.
```
10chemparm.pm.pna.in
```

OH lookup tables: not used when using micro-CB-IV.
```
00oh.lowr.dat
00oh.uppr.dat
```

Photolysis rate lookup table. Supplied with the model. NOTE: not to be altered by the user.
```
13photrk.dat
```

Meteorological input files generated by meteorological model output processor (e.g., processing of MM5 model outputs).
```
14wind.36km.960616.12lyr.1hr.bin
15press.36km.960616.12lyr.1hr.bin
16temp.36km.960616.12lyr.1hr.bin
17hum.36km.960616.12lyr.1hr.humfix.bin
55clw.36km.960616.12lyr.1hr.bin
56rnw.36km.960616.12lyr.1hr.bin
```

Land use file typically generated from USGS land use data. Please see manual for format details.
```
18remsad.36km_lu.full.bin
```

Surface chlorine concentration file. Used only when running mercury chemistry. Please refer to manual.
```
29cl2rems.prn
```
Average terrain elevations, usually derived from meteorological model data sets.
```
19remsad.36km.dummy_terrain.bin
```
Elevated point source file typically generated by emissions processing software (e.g., EPS2, SMOKE, EMS) and the point source preprocessor (e.g., PTSRCE).
```
20ptsrce.camd.base96.pm.us+can+mx.sum.$dofw.a0
```

Low-level emission files for weekdays, Saturday, and Sunday, generated by emissions processing software (e.g., EPS2, SMOKE, EMS).
```
21emiss.all.camd.base96.pm.jun.wkd.a0
22emiss.all.camd.base96.pm.jun.sat.a0
23emiss.all.camd.base96.pm.jun.sun.a0
```

Initial conditions for species concentrations generated by AIRQUAL processor.
```
24ic.remsad.36km_12lyr.const.new_bt2_hg.bin
```

Ozone lookup table, not used when running micro-CB-IV.
```
00/dev/null
```

Meteorological input files generated by meteorological model output processor (e.g., processing of MM5 model outputs).
```
26precip.36km.960616.12lyr.1hr.binnew
27kv.36km.960616.12lyr.1hr.min1.bin
```

Space for fine grid meteorological files. If no fine grid met files are used, the models interpolates from the coarse grid files.
```
00/dev/null
00/dev/null
00/dev/null
00/dev/null
```

Land use file for fine grid, typically generated from USGS land use data. Please see manual for format details.
```
90sfc.ladco.12km.nhd.bin
```

Fine grid low-level emission files for weekdays, Saturday, and Sunday, generated by emissions processing software (e.g., EPS2, SMOKE, EMS).
```
41emiss.all.ladco.base96.pm.jun.wkd.a0
71emiss.all.ladco.base96.pm.jun.sat.a0
72emiss.all.ladco.base96.pm.jun.sun.a0
```

Lateral boundary conditions generated by BOUNDARY processor.
```
28bc.remsad.36km_12lyr.const.new_bt2_hg.bin
```

Optional dry deposition velocity file. If no file is supplied, the model calculates dry deposition velocities internally.
```
00depovel.bin
```

Coarse grid instantaneous file for restart.
```
atdm.0615.$scen[$j].inst
```

Fine grid instantaneous file for restart.
```
$OUTDIR/INST/atdm.0615.$scen[$j].finst

-eof-
#
```

5. REMSAD OUTPUT FILES

REMSAD output files include both formatted, ASCII and unformatted, binary files. The formatted output files reiterate the simulation control parameters, provide information to the user on the progress of the simulation, and contain summaries various input and simulation variables for checking the behavior of the simulation as well as any diagnostic messages. The unformatted files contain simulated concentrations or mass totals of selected REMSAD species for analysis and use in restarting the model.

For ease of reading, all exhibits follow the text of this section.

5.1. Formatted Output

Formatted, ASCII REMSAD output files include the standard output file (SYSOUT), simulation trace output (SIMOUT), and diagnostic output (DIAG).

5.1.1. Standard Output File (SYSOUT)

The standard output file contains all of the computer system messages as well as the information written by REMSAD to the standard I/O file unit number. Assignment of the actual unit number is determined by the computer operating system. This file primarily summarizes operational status and timing information for the simulation. A sample of the information written to the SYSOUT file during an REMSAD simulation is shown in Exhibit 5-1.

The first line of the example notes the version of the model in use. The next 200 or so lines track initialization of the model. A warning message regarding the number of cells in the PTSOURCE file may in general be ignored since the values are not used by the model. The user, however, should make a habit of reviewing the warning messages to determine if the correct input file has been designated.

The input species list is mapped to the internal species list at "1". The order of the internal species list is established in the CHEMPARAM file. Note that this ordering may be different in input data files. The model reorders the species internally to match the order in the CHEMPARAM file.

Beginning at "2", the species read from data files and the time intervals read from the files are summarized. The number of point sources read (NOPTS) is written along with the unit number from which point source data are read at "3". Information about species read from the low-level emissions file follows and then information about time intervals read from various input data files.

NOTE

Dates on the emission input files are not required to match the modeled dates when the one-day emission input flag is true.

Steps in the initialization process are noted in lines beginning at "4'. The time step selection line gives the current date and time, the time step (minutes) selected for use on the coarse grid, the print or data interval (whichever is smaller), and the calculated maximum allowable step sizes (minutes) for horizontal advection and horizontal diffusion.

The lines following "5" tally the number of cells that have surface emissions for each of the species in the simulation. At "6", the number of point sources emitting each species is listed. At "7", ("Levels:") the distribution of point sources according to the vertical layer into which emissions are injected is given.

NOTE

The number of point sources listed at "7" may differ from that listed earlier. This difference is due to the fact that some sources may be located in boundary cells and therefore are not included in the calculations.

Messages written to standard output from this point onward summarize progress of the simulation through the various steps of the solution. Calls to various subroutines are noted. In the note after EMCORS concentrations for all simulated species at a single cell in the domain is output to the SYSOUT file. The output prints additional diagnostics on the concentrations as various steps are completed in the simulation.

At "8" timing information in CPU seconds for the step just completed for the fine grids is provided. Various parameters developed in the cloud diagnosis and samples of the input and output of the sulfate routine are noted in the output.

In the line for AVERAG at "9", the numbers are time [130.00], date [980101], δ-time for the time step [30.0], and a flag to the averaging routine. This flag indicates the type of processing for calculating the running average. The values of m indicate:

        m = 1 initialize average
        m = 2 continue average
        m = 3 complete average for output interval.

Finally, at "10", the CPU time used for the entire time step is summarized. Total elapsed time is the total time used thus far in the simulation. Times are then broken down for subsections of the solution.

After "11', lines begin to repeat information for the next time step. This information continues to be printed for the duration of the simulation.

5.1.2. Simulation Trace Output (SIMOUT)

The SIMOUT file includes some output that is also included in the standard output file as well as the diagnostic output file. The name and unit number for this file are specified in REMSAD simulation control input. An example of the SIMOUT file is shown in Exhibit 5-2.

The first line in the example document prints the run identification text. Starting at "1", the time-span of the simulation is documented. At "2", the modeling grid definition is printed. Definition of the model layers (the sigma levels) is documented for each of the grids starting at "3". Model options selected in the run are printed starting at "4". Beginning at "5", the diagnostic information included in the standard output that tracks the CPU time used is reiterated. This CPU time information continues to be written to this file during the course of the simulation.

5.1.3.   Diagnostic Output (DIAG)

The diagnostic file provides summary information about data that have been read by the model and also includes tables of mass flux. The filename and unit number for the DIAG file is specified in the REMSAD simulation control input file. An example of a DIAG file is shown in Exhibit 5-3.

Starting at the point labeled "1" to the point labeled "2" in the example, the simulation options and some of the data files used are documented. Starting at "2", the chemistry parameter inputs are echoed to the file. At "3", maps are printed summarizing the grid configuration. Each digit in the maps represents a coarse grid cell. A line is written for each row in the domain, but because of line length limitations the lines sometimes wrap to the beginning of the next line. The first map shows the nesting ratio for each fine grid. A "0" indicates that the cell is a coarse grid cell only, a "3" would indicate that this coarse grid cell is covered by a fine grid that is sub-divided at a 3 to 1 ratio. The next map shows the id nos. used by the model for each fine grid. A zero again indicates a cell that is coarse grid only. The number at other locations indicates the fine grid no. that the model uses to refer to the grid that covers this cell. For grids nested at multiple levels, the finest grid id no. will be shown. After the maps, more of the data files used in the simulation are documented.

At "4", data regarding point sources are tabulated. In the example, the data are tabulated for only the first five sources.

After the information on point sources, emissions totals are included for each grid and each species for both area and point sources. Following these totals, the concentrations at the top of the region, the definition of boundary cells, and the initial concentrations (at "5") are documented. The concentrations at the top of the region and initial conditions are given in parts per million.

Beginning at "6", the minimum, maximum, and average values of many input variables are tabulated. Included are most meteorological variables and boundary concentrations. This table is repeated each time the input data is updated. It lists:

boundary concentrations ($\mu mol/m^3$)	u-, v-wind components (m/s)
absolute value of the v-component	total wind speed (m/s)
surface pressure (mb)	height (m)
horizontal diffusivity (km^2/min)	vertical diffusivity (m^2/s)
temperature (K)	H_2O concentration (g/g)
cloud cover (%)	O_3 concentration (ppm)
rain fall (in/hr)	deposition velocity (m/s)

At the point marked "7", the mass flux summary is printed for the fine grids and then for the coarse grid. Since this simulation began at 0100, the mass flux values at 0100 are zero. Therefore, most of these lines are skipped in the example. The tabulation of input values for the following hour and the mass flux summary for 0400 would begin next. All values in these summaries are in moles and cover the time period from the last print up to the time at the beginning of the table. The species included in the summary are those listed in the control file to be saved to the AVERAGE file. The summaries for each of the fine grids are first, followed by a summary for the coarse grid. At the end of the simulation, a cumulative summary is printed covering the entire span of the run.

All fluxes for a given species are grouped together. On the left side of the summary, the fluxes across each of the boundary surfaces of the grid are tabulated. Fluxes are included for each of the vertical surfaces that define the boundaries of the grid, as is the flux across the horizontal

surface that defines the top boundary of the grid (note: all fluxes across the top are zero). For each surface the total flux into the grid, out of the grid, and the net flux is printed. Fluxes in and out are always expressed as positive numbers. The net flux is positive if there is an addition of mass to the grid or negative if mass is removed.

On the right side of the summary, the mass added to the grid through emissions is summarized. Mass lost to surface deposition is also tabulated. Finally, the "Tot mass" line gives the total number of moles of the species in the grid at the current time. For the coarse grid, the emissions summary includes all emissions in the region whether located within a fine grid or not.

5.2. Unformatted output

Some concentrations are output as micrograms per cubic meter ($\mu g/m^3$). These concentrations can be converted to parts per million (ppm) as follows. The density of air at STP is 1293 g/m^3 and the average molecular weight of air is approximately 28.8 g/mol. Therefore, we have 44.9 mol/m^3 at STP. Hence,

$$(C \text{ in ppm}) = ((C \text{ in } \mu g/m^3)(\text{moles/g}))/(44.9 \text{ mol/m}^3)) \, (T/273) \, (1/P)$$

where T is the ambient temperature in Kelvin and P is pressure in atmospheres. This conversion can be accomplished using the REMSAD input data files to get the appropriate temperature and pressure.

Other concentrations are output as parts per million (ppm) and are easily converted to micrograms per cubic meter ($\mu g/m^3$) by multiplying by the appropriate molecular weight.

5.2.1. Coarse-Grid Average Concentration File

The coarse-grid AVERAGE file is a binary file containing averaged concentrations (in $\mu g/m^3$) of each of the species requested in the control file. The concentrations represent a running average over the output time interval specified by the user. This file is designated on record 3 of the REMSAD control input file. The file structure includes header records, time-invariant records, and time-varying records. This file structure is common to all unformatted output files. The REMSAD coarse-grid AVERAGE file includes concentrations for only layer 1. For examination of the three-dimensional structure of the concentration fields, the user should employ the instantaneous concentration files.

The AVERAGE file contains time-averaged concentrations for each species (specified in the control input file) in each grid cell for the entire modeling region. The contents of the unformatted AVERAGE is described in Table 5-1.

5.2.2. Nested-Grid(s) Average Concentration File

This is a single binary file containing average concentrations for all nested grids included in the simulation. The concentrations ($\mu g/m^3$) of each species requested in the control file are included for layer 1 only. To obtain data on the vertical structure of the predicted concentration fields, the user should utilize the instantaneous concentration file. The structure of the nested-grid file is described in Table 5-2.

5.2.3. Coarse-Grid Deposition File

The coarse-grid DEPOSITION file is a binary file containing deposition of each of the species requested in the control file. This file is designated on record 5 of the REMSAD control input file. The format of the file is the same as the format of the AVERAGE file. The file structure includes header records, time-invariant records, and time-varying records.

The DEPOSITION file contains total deposition for the output interval (g/km^2) for each species (specified in the control input file) in each grid cell for the entire modeling region. The contents of the unformatted DEPOSITION file is described in Table 5-3.

5.2.4. Nested-Grid(s) Deposition File

This is a single binary file containing predicted deposition for all nested grids included in the simulation (designated in the REMSAD control file). The deposition (g/km^2) of each species requested in the control file is included on the file. The structure of the nested-grid DEPOSITION file is described in Table 5-4.

5.2.5. Coarse-Grid Instantaneous Concentration File

The coarse-grid INSTANT file includes concentrations for all species in the simulation in parts per million (ppm). This file is designated on record 6 of the REMSAD control file. The full three-dimensional array of coarse-grid cells is included. The structure of the coarse-grid INSTANT file is given in Table 5-5.

The INSTANT file contains predicted concentration values as a function of time for each species over the region (x,y,z). The instantaneous values represent the concentration of each species at the end of the last time step before an output time interval is detected.

5.2.6. Nested-Grid(s) Instantaneous Concentration File

This file contains predicted concentrations (ppm) for all species in the simulation for all nested grids. This binary file (designated on record 8 or the REMSAD control file) includes concentrations for all layers in parts per million.

The structure of the nested-grid INSTANT file is described in Table 5-6.

5.2.7. Tagging Results

The results for the tagged species are written to the concentration and deposition files described above along with all other species. Each tagged species can be referenced in by the appropriate species name (e.g., HG0-1) to prepare output displays of that species. By the careful definition of the tagged species and the associated inputs (as described in section 2), displays of the tagged species can be prepared to show the total deposition of mercury (or cadmium) from a particular source type or geographic area. However, the mechanics of extracting the tagged species from the output files or preparing the displays is the same as for other species.

Exhibit 5-1.
Sample ATDM standard output file.

```
start model simulation ATDM v7.02, 07/16/02
 open input files
opening control file atdmin.0101.1998.a0
 initialize model
 Micro CB4 mechanism has been specified; you do not need lower OH lookup table.
 Micro CB4 mechanism has been specified; you do not need upper OH lookup tables.
 Micro CB4 mechanism has been specified;
 you need a look-up table for photolysis rate
 Micro CB4 mechanism has been specified; you do not need O3 file.
 before chread
 entered chread
 nspec1, nreact            22            77
 NSPEC =           36
 within chread, mxgas, nspint=          70         118
 mxgas=           70
Input species #   1 labelled NO        mapped to int[ 1 ]l species #   1
 within chread, mxgas, nspint=          70         118
 mxgas=           70
     ...
     ...
     ...
Input species #  36 labelled PMCOARS   mapped to internal species #  80
 ngas =          17npart=           10
 after allrate
  9.9999997E-06          5  4.9999999E-03
 120
 before 2
 before 3
 After 7, nncd =           0
 kcd:          0          0          0          0          0          0
         0          0          0          0
 end of chread and ngas is =          17
 after chread
 read surf file       140        104        11
 read terrain file       140        104
 read all of input file
 all species
Species   1 NO        on PTSOURCE file = speci[ 2 ]1 N        internally.
     ...
 Species  15 CARB        on PTSOURCE file = species    5 CARB        internally.
 hedpts nopts when read=        38326
 hedpts nopts at the end=        38326
 reading point source data nopts=[ 3 ]38326        20
 finish reading points
 in setup nopts =       38326
 Species   1 NO        on EMISSIONS file = species    1 NO        internally.
     ...
 Species  17 TERP        on EMISSIONS file = species   17 TERP        internally.
 in getqar       96015  1.000000         96015  4.000000
 Read interval    96015       1.00 to    96015       4.00 on unit    21
 in getqar       96015  1.000000         96015  4.000000
 Read interval    96015       1.00 to    96015       4.00 on unit    41
 in getqar       96015  1.000000         96015  4.000000
 Read interval    96015       1.00 to    96015       4.00 on unit    42
```

```
in getqar         96015   1.000000            96015    4.000000
Read interval     96015      1.00 to     96015      4.00 on unit   43
in getqar         96015   1.000000            96015    4.000000
Read interval     96015      1.00 to     96015      4.00 on unit   44
in getqar         96015   1.000000            96015    4.000000
Read interval     96015      1.00 to     96015      4.00 on unit   45
in getqar         96015   1.000000            96015    4.000000
Read interval     96015      1.00 to     96015      4.00 on unit   46
in getqar         96015   1.000000            96015    4.000000
Read interval     96015      1.00 to     96015      4.00 on unit   47
in getqar         96015   1.000000            96015    4.000000
Read interval     96015      1.00 to     96015      4.00 on unit   48
Read interval     96351      1.00 to     96351      4.00 on unit   20
nopts before the read of nn        38326
nemit =          15        38326        80       67000       120
call grdsp
deltax(1), deltay:    57.95439        41.11951
ifine, delfx(1,ifine), delfy(ifine):
         1   18.51727       13.70650
ifine, delfx(1,ifine), delfy(ifine):
         2   18.15401       13.70650
ifine, delfx(1,ifine), delfy(ifine):
         3   18.85273       13.70650
ifine, delfx(1,ifine), delfy(ifine):
         4   18.85273       13.70650
ifine, delfx(1,ifine), delfy(ifine):
         5   15.51193       13.70650
ifine, delfx(1,ifine), delfy(ifine):
         6   17.12794       13.70650
ifine, delfx(1,ifine), delfy(ifine):
         7   15.77151       13.70650
ifine, delfx(1,ifine), delfy(ifine):
         8   14.88377       13.70650
File on unit 24 is AIRQUALITY
Species   1 NO        on AIRQUALITY file = species   1 NO        internally.
    ...
start of hedibc and bnddef
File on unit 28 is BOUNDARY
Species   1 NO        on BOUNDARY   file = species   1 NO        internally.
    ...
enter update
enter update      100.0    980101(   98001)
read iwind        100.0    980101     100.0    980101
lfirst= T
in surface pressure file   100.0000         980101
read prs          100.0    980101     100.0    980101
kntmix=          1
lfirst= T
read prs          100.0    980101     100.0    980101
in surface pressure file   400.0000         980101
read prs          400.0    980101     100.0    980101
read temp         100.0    980101     100.0    980101
read water        100.0    980101     100.0    980101
before fgrtrp
in update and reading cloud water
read cloud water     100.0    980101     100.0    980101
read rain water      100.0    980101     100.0    980101
```

```
read rainfall        100.0     980101       100.0      980101
Read interval    98001       1.00 to      98365      24.00 on unit    28
read kv          100.0     980101       100.0     980101
end of diagn-2
Returned from update
idiag            0
before 206
after 206
after 207
end of setup
numfin =           8
lrstrt=  F ... calling finfil
tot mass by spec:  2.656E-01 2.656E+05 9.029E+08 2.656E+05 2.656E+03 2.656E+03
 2.656E+00 2.656E+05 2.629E+09 1.935E+04 1.328E+07 1.328E+07
 2.656E+03 2.656E+03 2.656E+03 0.000E+00 2.656E+03 2.656E+03
 2.656E+03 2.656E+03 2.656E+03 2.656E+03 2.656E+03 2.656E+03
 2.656E+03 2.656E+03 2.656E+03
     ...
within prtint-coarse grid       980101  0.9990000          980101   1.001000
within prtint-fine grid   100.0000          980101
end of prtint
after prtint
just enter surlyr routine
TIME STEP SELECTION AT       100.0     980101:       30.0    4    180.00        0.00
model initialized cpusecs=       26.0
ENTER AVERAG       100.0     980101      30.00  m =    1
Inside 330 loop, coldg,molwt,conc,mfac:
        31           67           1  1.1673574E-08   30.00000
 1.0000001E-11   2.5699072E-02
     ...
Inside 330 loop, coldg,molwt,conc,mfac:
        31           67          27  3.8911912E-06   1.000000
 1.0000000E-07   2.5699072E-02
enter avergf       100.0     980101       0.00  m =    1
enter avergf       100.0     980101       0.00  m =    1
enter avergf       100.0     980101       0.00  m =    1
enter avergf       100.0     980101       0.00  m =    1
enter avergf       100.0     980101       0.00  m =    1
enter avergf       100.0     980101       0.00  m =    1
enter avergf       100.0     980101       0.00  m =    1
enter avergf       100.0     980101       0.00  m =    1
conc:  1.0000001E-11  1.0000001E-05  3.4000002E-02  1.0000001E-05
 1.0000000E-07  1.0000000E-07  1.0000000E-10  1.0000001E-05  9.9000007E-02
 7.2880005E-07  5.0000002E-04  5.0000002E-04  1.0000000E-07  1.0000000E-07
 1.0000000E-07  0.0000000E+00  1.0000000E-07  1.0000000E-07  1.0000000E-07
 1.0000000E-07  1.0000000E-07  1.0000000E-07  1.0000000E-07  1.0000000E-07
 1.0000000E-07  1.0000000E-07  1.0000000E-07
 it1 ... timlft :         1   30.00000
     ...
 area sources:        10983          0        0    5    10983      10983
     10983          0          0      10983          0          0
         0          0      10983          0      10983      10983
     10983      10983          0          0          0      10983
     10983      10983      10983      10983
 points:        38210          0      0    38    6    38210      38210
     38210          0          0      38210          0          0
         0          0      38210          0          0      38210
```

```
     38210         38210             0              0              0        38210
     38210         38210         38210          38210
  levels:          2169          17102         175◄───────────────  7         51
           1             0             0              0              0             0
           0             0             0              0
 finished emcors
 conc:    2.4930824E-04  2.6031150E-05  3.4000002E-02  2.6031150E-05
  1.0243435E-04  1.3575486E-03  1.0000000E-10  1.0000001E-05  0.1025692
  7.2880005E-07  5.0000002E-04  5.0000002E-04  1.0000000E-07  3.8302169E-05
  1.0000000E-07  3.3094204E-04  6.2506465E-04  1.0932575E-07  1.1141346E-07
  1.0000000E-07  1.0000000E-07  1.0000000E-07  7.1624765E-04  5.2945851E-03
  1.2039971E-03  7.8919204E-03  1.9236693E-02
   it2 ... timlft1 :          1   15.00000
      ...
before vrtdif-1
 after vrtdif-1
 conc:    1.2574955E-04  1.7848835E-05  3.2460164E-02  1.7848835E-05
  5.1636973E-05  6.8470719E-04  1.0000000E-10  9.8928722E-06  0.1008003
  7.2096407E-07  4.7406537E-04  2.6393117E-04  1.0000000E-07  1.8947278E-05
  1.0000000E-07  1.7160780E-04  2.6733970E-04  1.0034118E-07  1.0561444E-07
  9.6799241E-08  9.5795841E-08  9.8312498E-08  3.5696069E-04  2.6383915E-03
  6.2047585E-04  4.0507708E-03  6.7399801E-03
 before stepz
 after stepz
 conc:    1.2198719E-04  1.7314809E-05  3.1488977E-02  1.7314809E-05
  5.0092025E-05  6.6422118E-04  1.0000000E-10  9.5968835E-06  9.7784422E-02
  6.9939324E-07  4.5988162E-04  2.5603452E-04  9.7008062E-08  1.8380386E-05
  1.0000000E-07  1.6647339E-04  2.5934106E-04  9.7849778E-08  1.0246129E-07
  9.4270021E-08  9.3417306E-08  9.5557681E-08  3.4741542E-04  2.5678398E-03
  6.0207385E-04  3.9322432E-03  6.7520337E-03
 before 5003
 enter stepx_04        15.00
 enter stepy_04        15.00
 end of stepy04
 finished stepxy
 conc:    1.3106708E-04  1.8472001E-05  3.2149490E-02  1.8472001E-05
  5.8484457E-05  7.7577273E-04  1.0223345E-10  9.8110440E-06  0.1002512
  7.1500142E-07  4.6911874E-04  2.5421334E-04  9.9169021E-08  2.0132198E-05
  1.0223346E-07  1.7006180E-04  2.6746994E-04  1.0045292E-07  1.0540526E-07
  9.6258638E-08  9.5349989E-08  9.7633368E-08  4.1640166E-04  3.0385237E-03
  7.1206089E-04  4.4610058E-03  7.0931129E-03
      ...


                                                       8
completed fine grids in       ◄───────────  3 passes.
 elapsed time for fine grid operations:
diffsf                    0.06
 timestep loop         92.65
   fvrtwd/emfine/fbdfil/htfnew    0.52
   stepxyf                        7.99
   stepzf                         4.39
   fvrtdif                        5.50
   rchemf                        40.79
 crsfil                    0.38
 total elapsed for each nested grid:
        1          4.41
        2         27.29
```

```
          3         9.19
          4          0.35
          5         10.17
          6         56.43
          7         21.85
          8          2.48
after fine grids
enter rchem2      30.00
Average cloud =   0.3701663
Average fnonpr =   0.2803611
Number of zero cloud =       262780
Number of zero fnonpr =        4368
sulfate in: SO2,GSO4,ASO4,H2O2,O3,rsulf,clwc
 1.0141066E-07  9.9900902E-08  9.9899765E-08  4.9950095E-04  3.3965841E-02
 3.6948222E-13  1.0000000E-07
bsulf,wsulf,sulfw,sulfg
 0.0000000E+00  9.3868033E-09  9.3868033E-09  3.6948222E-13
sulfate out: SO2,GSO4,ASO4,H2O2,O3,so2av
 9.2023853E-08  9.9901271E-08  1.0928657E-07  4.9949164E-04  3.3965841E-02
 7.2088540E-08
Average cloud =   0.3968549
Average fnonpr =   0.4089714
Number of zero cloud =       70840
Number of zero fnonpr =        3936
     ...
cpumar =   34.17760
conc:   3.9544396E-11  1.4505678E-04  3.2012615E-02  1.4731839E-04
 6.3628788E-05  7.8625558E-04  7.9799281E-07  1.0205413E-05  0.1002506
 7.1497777E-07  4.6914781E-04  2.5462321E-04  9.3614057E-07  2.0131554E-05
 1.0287904E-07  1.6640135E-04  2.6724456E-04  1.2927982E-08  1.0605083E-07
 9.6258645E-08  1.2927982E-08  4.0547860E-07  4.1640166E-04  3.0385237E-03
 7.1206095E-04  4.4610058E-03  7.0931134E-03
before stepx
enter stepx_04      15.00
enter stepy_04      15.00
end of stepy04
conc:   4.3347454E-11  1.5516230E-04  3.2699615E-02  1.5760449E-04
 7.1871182E-05  8.9214509E-04  8.3091231E-07  1.0437708E-05  0.1028025
 7.3121396E-07  4.7894969E-04  2.5302361E-04  9.7019426E-07  2.1850426E-05
 1.0525808E-07  1.7003375E-04  2.7349070E-04  1.2691783E-08  1.0912818E-07
 9.8319418E-08  1.2691783E-08  4.1560648E-07  4.8030898E-04  3.4849152E-03
 8.1609213E-04  4.9734581E-03  7.4391938E-03
before continue 6003            1          15
after 6013
before stepz
conc:   4.2050523E-11  1.5051993E-04  3.1721260E-02  1.5288906E-04
 6.9720838E-05  8.6545263E-04  8.0605190E-07  1.0125418E-05  9.9726737E-02
 7.0933646E-07  4.6461981E-04  2.4545330E-04  9.4116660E-07  2.1196674E-05
 1.0210882E-07  1.6494644E-04  2.6530802E-04  1.2376655E-08  1.0587012E-07
 9.5750472E-08  1.2376655E-08  4.0395597E-07  4.6746532E-04  3.3917271E-03
 7.9188851E-04  4.8279325E-03  7.4530435E-03
before vrtdif
after vrtdif
conc:   3.2433865E-11  1.1453344E-04  3.0957084E-02  1.1643095E-04
 5.1931653E-05  6.4449396E-04  5.6495355E-07  9.9580802E-06  9.9123605E-02
 7.0470816E-07  4.5147233E-04  1.9317301E-04  7.2647441E-07  1.5112714E-05
 1.0229692E-07  1.2242922E-04  1.7177702E-04  9.9402593E-09  1.0357714E-07
```

```
 9.3574755E-08  9.9402593E-09  3.9499074E-07  3.3664628E-04  2.4299617E-03
 5.8099721E-04  3.5369566E-03  4.2766929E-03
  it1 ... timlft :        2  0.0000000E+00
conc:  3.2433865E-11  1.1453344E-04  3.0957084E-02  1.1643095E-04
 5.1931653E-05  6.4449396E-04  5.6495355E-07  9.9580802E-06  9.9123605E-02
 7.0470816E-07  4.5147233E-04  1.9317301E-04  7.2647441E-07  1.5112714E-05
 1.0229692E-07  1.2242922E-04  1.7177702E-04  9.9402593E-09  1.0357714E-07
 9.3574755E-08  9.9402593E-09  3.9499074E-07  3.3664628E-04  2.4299617E-03
 5.8099721E-04  3.5369566E-03  4.2766929E-03
ENTER AVERAG      130.0    980101      30.00   m =        9
Inside 105 loop, avcong, deltat, coldg:
         31          67          1  1.7510361E-07   30.00000
 1.1673574E-08
Inside 105 loop, avcong, deltat, coldg:
         31          67          2  0.2684922      30.00000
 1.7899482E-02
Inside 105 loop, avcong, deltat, coldg:
         31          67          3  952.5636       30.00000
  63.50424
Inside 105 loop, avcong, deltat, coldg:
         31          67          4  0.2684922      30.00000
 1.7899482E-02
     ...
Inside 285 loop, avcong, deltat, molwt:
         31          67          1  7.4281922E-07   30.00000
  30.00000
conc, mfac:
 3.2433865E-11  2.5708715E-02
Inside 285 loop, avcong, deltat, molwt:
         31          67          2  3.342472       30.00000
  46.00000
conc, mfac:
 1.1453344E-04  2.5708715E-02
Inside 285 loop, avcong, deltat, molwt:
         31          67          3  1819.550       30.00000
  48.00000
conc, mfac:
 3.0957084E-02  2.5708715E-02
Inside 285 loop, avcong, deltat, molwt:
         31          67          4  3.393400       30.00000
  46.00000
conc, mfac:
 1.1643095E-04  2.5708715E-02
     ...
Inside 330 loop, coldg,molwt,conc,mfac:
         31          67          1  3.7847705E-08   30.00000
 3.2433865E-11  2.5708715E-02
Inside 330 loop, coldg,molwt,conc,mfac:
         31          67          2  0.2049320      46.00000
 1.1453344E-04  2.5708715E-02
Inside 330 loop, coldg,molwt,conc,mfac:
         31          67          3  57.79908       48.00000
 3.0957084E-02  2.5708715E-02
Inside 330 loop, coldg,molwt,conc,mfac:
         31          67          4  0.2083272      46.00000
 1.1643095E-04  2.5708715E-02
     ...
```

```
before 93
 End dt:  130.0 980 01  30.00
 Total elapsed time=          140.0 This time step= 113.97
 vertwd/emcors/hgtnew     0.11
 bdrfil                   0.08
 stepxy                   4.93
 stepz                    3.78
 vrtdif                   4.93
 rchem                   40.13
 averag                   0.05
 update/surlyr            0.00
 rd ems/printr/averg      0.00
xfine     59.70
 conc:   3.2433865E-11  1.1453344E-04  3.0957084E-02  1.1643095E-04
  5.1931653E-05  6.4449396E-04  5.6495355E-07  9.9580802E-06  9.9123605E-02
  7.0470816E-07  4.5147233E-04  1.9317301E-04  7.2647441E-07  1.5112714E-05
  1.0229692E-07  1.2242922E-04  1.7177702E-04  9.9402593E-09  1.0357714E-07
  9.3574755E-08  9.9402593E-09  3.9499074E-07  3.3664628E-04  2.4299617E-03
  5.8099721E-04  3.5369566E-03  4.2766929E-03
   it1 ... timlft :          1   30.00000
 conc:   3.2433865E-11  1.1453344E-04  3.0957084E-02  1.1643095E-04
  5.1931653E-05  6.4449396E-04  5.6495355E-07  9.9580802E-06  9.9123605E-02
  7.0470816E-07  4.5147233E-04  1.9317301E-04  7.2647441E-07  1.5112714E-05
  1.0229692E-07  1.2242922E-04  1.7177702E-04  9.9402593E-09  1.0357714E-07
  9.3574755E-08  9.9402593E-09  3.9499074E-07  3.3664628E-04  2.4299617E-03
  5.8099721E-04  3.5369566E-03  4.2766929E-03
 area sources:         10983          0          0      10983      10983
       10983          0          0      10983          0          0
           0          0      10983          0      10983      10983
       10983      10983          0          0          0      10983
       10983      10983      10983      10983
 points:         38210          0          0      38210      38210
       38210          0          0      38210          0          0
           0          0      38210          0          0      38210
       38210      38210          0          0          0      38210
       38210      38210      38210      38210
 levels:          2169      17102      17594       1293         51
           1          0          0          0          0          0
           0          0          0          0
finished emcors
```

10

11

Exhibit 5-2.
Sample ATDM simulation Trace Output.

```
ATDM PM Run: jan 1, src7.02: Micro Mech Chemistry with ISOP&TERP


  Simulation start time/date:                100.    ┌─── 1 ┐0101
  Simulation end time/date:                  100.       980102
  Data input interval:                                  300.
  Output interval:                                      300.
  Maximum coarse grid time step (min):                   30.

                                                    ┌─── 2 ┐
  Longitude grid spacing:                               56
  Latitude grid spacing:                               0.370
  Grid dimensions (x-, y-, z-cells):     140  104   15
  Number of species:                                    27

  Longitude of western boundary:            -138.00
  Longitude of eastern boundary:             -60.16
  Latitude of southern boundary:              20.11
  Latitude of northern boundary:              58.58
  time zone:                                   5.0  ┌─── 3 ┐
  Model top pressure (mb):                     100
  Surface:          Sigma:  1.000
  Top of Layer:  1  Sigma:  0.996
  Top of Layer:  2  Sigma:  0.988
  Top of Layer:  3  Sigma:  0.965
  Top of Layer:  4  Sigma:  0.916
  Top of Layer:  5  Sigma:  0.866
  Top of Layer:  6  Sigma:  0.812
  Top of Layer:  7  Sigma:  0.748
  Top of Layer:  8  Sigma:  0.656
  Top of Layer:  9  Sigma:  0.554
  Top of Layer: 10  Sigma:  0.449
  Top of Layer: 11  Sigma:  0.354
  Top of Layer: 12  Sigma:  0.260
  Top of Layer: 13  Sigma:  0.172
  Top of Layer: 14  Sigma:  0.087
  Top of Layer: 15  Sigma:  0.000
  Fine Grid #:    1
  Surface:          Sigma:  1.000
  Top of Layer:  1  Sigma:  0.996
  Top of Layer:  2  Sigma:  0.988
  Top of Layer:  3  Sigma:  0.965
  Top of Layer:  4  Sigma:  0.916
  Top of Layer:  5  Sigma:  0.866
  Top of Layer:  6  Sigma:  0.812
  Top of Layer:  7  Sigma:  0.748
  Top of Layer:  8  Sigma:  0.656
  Top of Layer:  9  Sigma:  0.554
  Top of Layer: 10  Sigma:  0.449
  Top of Layer: 11  Sigma:  0.354
  Top of Layer: 12  Sigma:  0.260
  Top of Layer: 13  Sigma:  0.172
  Top of Layer: 14  Sigma:  0.087
```

```
 Top of Layer: 15   Sigma:  0.000
     ...
     ...
     ...
 Fine Grid #:   8
 Surface:           Sigma:  1.000
 Top of Layer:  1   Sigma:  0.996
 Top of Layer:  2   Sigma:  0.988
 Top of Layer:  3   Sigma:  0.965
 Top of Layer:  4   Sigma:  0.916
 Top of Layer:  5   Sigma:  0.866
 Top of Layer:  6   Sigma:  0.812
 Top of Layer:  7   Sigma:  0.748
 Top of Layer:  8   Sigma:  0.656
 Top of Layer:  9   Sigma:  0.554
 Top of Layer: 10   Sigma:  0.449
 Top of Layer: 11   Sigma:  0.354
 Top of Layer: 12   Sigma:  0.260
 Top of Layer: 13   Sigma:  0.172
 Top of Layer: 14   Sigma:  0.087
 Top of Layer: 15   Sigma:  0.000
        restart option =   F                                    ┌─────┐
dry deposition option =   T                                     │  4  │
wet deposition option =   T                                     └─────┘
      sediment option =   T
  PM chemistry option =   T
 TOX chemistry option =   F
 CB4 Mechanism option =   T
     cartesian option =   F
   area source option =   T
  point source option =   T
   1 day emiss option =   T
 1 day met inp option =   F
staggered wind option =   F
O3 and OH file option =   F
dtmin1=   0.000010 maxitr=      5 rerror=   0.005000
elapsed time for fine grid operations:                          ┌─────┐
diffsf                  0.06                                     │  5  │
timestep loop          92.65                                    └─────┘
  fvrtwd/emfine/fbdfil/htfnew   0.52
  stepxyf                       7.99
  stepzf                        4.39
  fvrtdif                       5.50
  rchemf                       40.79
crsfil                  0.38
total elapsed for each nested grid:
      1        4.41
      2       27.29
      3        9.19
      4        0.35
      5       10.17
      6       56.43
      7       21.85
      8        2.48

       time  130.00         totime   30.00         deltat   30.00
End dt:   130.0 980101   30.00
```

```
Total elapsed time=          140.0 This time step= 113.97
vertwd/emcors/hgtnew     0.11
bdrfil                   0.08
stepxy                   4.93
stepz                    3.78
vrtdif                   4.93
rchem                   40.13
averag                   0.05
update/surlyr            0.00
rd ems/printr/averg      0.00
        ...
        ...
        ...
elapsed time for fine grid operations:
diffsf                   0.05
timestep loop           74.54
  fvrtwd/emfine/fbdfil/htfnew    0.42
  stepxyf                        7.16
  stepzf                         3.74
  fvrtdif                        5.45
  rchemf                        38.85
crsfil                   0.38
total elapsed for each nested grid:
        1        1.54
        2       26.13
        3        3.11
        4        0.29
        5        9.05
        6       22.29
        7       27.18
        8        3.92


       time  100.00           totime 2400.00           deltat    30.00
End dt:   100.0 980102   30.00
Total elapsed time=        5451.1 This time step= 118.87
vertwd/emcors/hgtnew     0.11
bdrfil                   0.08
stepxy                   5.40
stepz                    3.77
vrtdif                   5.04
rchem                   41.00
averag                   0.06
update/surlyr            0.00
rd ems/printr/averg      7.29
```

Exhibit 5-3.
Sample ADTM diagnostic file.

```
open unit=67  file=/m2/remsadow/big_run/output/jan/AVRG/   0101.1998.a0.avrg
for average conc output                                    1
 open unit=69  file=/m2/remsadow/big_run/output/jan/DEPN/atdm.0101.1998.a0.depn
for deposition output
 open unit=51  file=/m2/remsadow/big_run/output/jan/INST/atdm.0101.1998.a0.inst
for dump (inst) conc out
 open unit=68 file=/m2/remsadow/big_run/output/jan/AVRG/atdm.0101.1998.a0.favrg
for fine grid average conc output
 open unit=70 file=/m2/remsadow/big_run/output/jan/DEPN/atdm.0101.1998.a0.fdepn
for fine grid deposition output
 open unit=52  file=/m2/remsadow/big_run/output/jan/INST/atdm.0101.1998.a0.finst
for fine grid inst conc output


 ATDM PM Run: jan 1, src7.02: Micro Mech Chemistry with ISOP&TERP



 Simulation start time/date:              100.        980101
 Simulation end time/date:                100.        980102
 Data input interval:                                 300.
 Output interval:                                     300.
 Maximum coarse grid time step (min):             30.

 Longitude grid spacing:                          0.556
 Latitude grid spacing:                           0.370
 Grid dimensions (x-, y-, z-cells):    140  104   15
 Number of species:                               27

 Longitude of western boundary:             -138.00
 Longitude of eastern boundary:              -60.16
 Latitude of southern boundary:              20.11
 Latitude of northern boundary:              58.58
 time zone:                               5.0
 Model top pressure (mb):                  100.00
 Surface:            Sigma:  1.000
 Top of Layer:  1    Sigma:  0.996
 Top of Layer:  2    Sigma:  0.988
 Top of Layer:  3    Sigma:  0.965
 Top of Layer:  4    Sigma:  0.916
 Top of Layer:  5    Sigma:  0.866
 Top of Layer:  6    Sigma:  0.812
 Top of Layer:  7    Sigma:  0.748
 Top of Layer:  8    Sigma:  0.656
 Top of Layer:  9    Sigma:  0.554
 Top of Layer: 10    Sigma:  0.449
 Top of Layer: 11    Sigma:  0.354
 Top of Layer: 12    Sigma:  0.260
 Top of Layer: 13    Sigma:  0.172
 Top of Layer: 14    Sigma:  0.087
 Top of Layer: 15    Sigma:  0.000
 Fine Grid #:   1
 Surface:            Sigma:  1.000
```

```
  Top of Layer:  1   Sigma:  0.996
  Top of Layer:  2   Sigma:  0.988
  Top of Layer:  3   Sigma:  0.965
  Top of Layer:  4   Sigma:  0.916
  Top of Layer:  5   Sigma:  0.866
  Top of Layer:  6   Sigma:  0.812
  Top of Layer:  7   Sigma:  0.748
  Top of Layer:  8   Sigma:  0.656
  Top of Layer:  9   Sigma:  0.554
  Top of Layer: 10   Sigma:  0.449
  Top of Layer: 11   Sigma:  0.354
  Top of Layer: 12   Sigma:  0.260
  Top of Layer: 13   Sigma:  0.172
  Top of Layer: 14   Sigma:  0.087
  Top of Layer: 15   Sigma:  0.000
      ...
      ...
      ...
  Fine Grid #:   8
  Surface:          Sigma:  1.000
  Top of Layer:  1   Sigma:  0.996
  Top of Layer:  2   Sigma:  0.988
  Top of Layer:  3   Sigma:  0.965
  Top of Layer:  4   Sigma:  0.916
  Top of Layer:  5   Sigma:  0.866
  Top of Layer:  6   Sigma:  0.812
  Top of Layer:  7   Sigma:  0.748
  Top of Layer:  8   Sigma:  0.656
  Top of Layer:  9   Sigma:  0.554
  Top of Layer: 10   Sigma:  0.449
  Top of Layer: 11   Sigma:  0.354
  Top of Layer: 12   Sigma:  0.260
  Top of Layer: 13   Sigma:  0.172
  Top of Layer: 14   Sigma:  0.087
  Top of Layer: 15   Sigma:  0.000
        restart option =  F
 dry deposition option =  T
 wet deposition option =  T
        sediment option =  T
   PM chemistry option =  T
  TOX chemistry option =  F
  CB4 Mechanism option =  T
      cartesian option =  F
    area source option =  T
   point source option =  T
    1 day emiss option =  T
  1 day met inp option =  F
 staggered wind option =  F
 O3 and OH file option =  F
  long/latitude coordinate system
 open unit=10  file=/m2/remsadow/big_run/extra/chemparm.pm.pna.in
for chem file
 open unit=13  file=/m2/remsadow/big_run/extra/photrk.dat
for photolysis data
 open unit=14  file=/m2/remsadow/metdata/jan/jan_out.wind
for wind file
```

```
 open unit=15  file=/m2/remsadow/metdata/jan/jan_out.press
for pressure file
 open unit=16  file=/m2/remsadow/metdata/jan/jan_out.temp
for temper file
 open unit=17  file=/m2/remsadow/metdata/jan/jan_out.humid
for water file
 open unit=55  file=/m2/remsadow/metdata/jan/jan_out.cwmr
for cloud water file
 open unit=56  file=/m2/remsadow/metdata/jan/jan_out.rwmr
for rain water file
 open unit=18  file=/m2/remsadow/big_run/extra/sfc.remsad.a0
for surf file
 open unit=29  file=/m2/remsadow/big_run/extra/cl2rems_a0.txt
for cl2 file
 open unit=19  file=/m2/remsadow/metdata/jan/jan_out.terrain
for terrain file
 open unit=20
file=/m2/remsadow/eps2/omef_all/ptsrce.base96.pm.us+can+mx.win.wkd.3hrblk
for pt ems file
 open unit=21
file=/m2/remsadow/eps2/omef_all/emiss.all.base96.pm.jan.wkd.3hrblk.r0.a0
for aem weekday file
 open unit=22
file=/m2/remsadow/eps2/omef_all/emiss.all.base96.pm.jan.sat.3hrblk.r0.a0
for aem saturday file
 open unit=23
file=/m2/remsadow/eps2/omef_all/emiss.all.base96.pm.jan.sun.3hrblk.r0.a0
for aem sunday file
 open unit=24  file=/m2/remsadow/big_run/extra/airqul.remsad.bin
for initial conditions
 open unit=26  file=/m2/remsadow/metdata/jan/jan_a0_out.precip
for rain file
 open unit=27  file=/m2/remsadow/metdata/jan/jan_a0_out.kv
for kv dif file


***************  CHEMPARAM FILE  *******************
File description header record
    File type        = CHEMPARAM
    File id          = CHEMISTRY PARAMETERS FOR ATDM V3.00, PM RUN with Micro C
B4 M
    No of species    = 36
    No of size dists =  9
Micro CB4 mechanism:
    No of species    = 22
    No of reactions  =  77
 Particulate size bins:
      0.022  0.071  0.141  0.316  0.707  1.581  3.536  7.071
 Mass fraction distributions
 #  1:  0.003  0.018  0.108  0.106  0.451  0.117  0.089  0.073
 Mass fraction > 1 um:  0.279
 #  2:  0.025  0.135  0.680  0.135  0.025  0.000  0.000  0.000
 Mass fraction > 1 um:  0.000
 #  3:  0.000  0.000  0.022  0.116  0.588  0.135  0.069  0.048
 Mass fraction > 1 um:  0.252
 #  4:  0.004  0.022  0.127  0.119  0.498  0.113  0.058  0.040
 Mass fraction > 1 um:  0.211
 #  5:  0.020  0.108  0.549  0.135  0.156  0.027  0.005  0.000
```

2

```
Mass fraction > 1 um:  0.032
#  6:  0.004  0.024  0.141  0.132  0.552  0.126  0.000  0.000
Mass fraction > 1 um:  0.126
#  7:  0.000  0.000  0.000  0.000  0.000  0.000  0.402  0.598
Mass fraction > 1 um:  1.000
#  8:  0.050  0.245  0.425  0.200  0.020  0.020  0.020  0.020
Mass fraction > 1 um:  0.060
#  9:  0.020  0.090  0.161  0.306  0.106  0.046  0.109  0.162
Mass fraction > 1 um:  0.317
Species parameters record
    Spec Name    React    SSIC    SSBC          Low Bd Num
    NO              T       F       F      1.0000E-12
    NO2S            T       F       F      1.0000E-09
    O3              T       T       T      1.0000E-09
    NO2             T       F       F      1.0000E-09
    CARB            T       F       F      1.0000E-07
    VOC             T       F       F      1.0000E-06
    PNA             T       F       F      1.0000E-10
    PAN             T       F       F      1.0000E-10
    CO              T       F       F      1.0000E-04
    HNO2            T       F       F      1.0000E-12
    H2O2            T       F       F      1.0000E-09
    HNO3            T       F       F      1.0000E-07
    NTR             T       F       F      1.0000E-10
    SO2             T       F       F      1.0000E-07
    SULF            T       F       F      1.0000E-07
    ISOP            T       F       F      1.0000E-12
    TERP            T       F       F      1.0000E-12
    SV1             T       F       F      1.0000E-20
    SV2             T       F       F      1.0000E-20
    SV3             T       F       F      1.0000E-20
    SV4             T       F       F      1.0000E-20
    NH3             F       F       F      1.0000E-20
    PNO3            1 1.000E+00 1.000E+00 1.000E-20
    GSO4            2 1.000E+00 1.000E+00 1.000E-20
    ASO4            3 1.000E+00 1.000E+00 1.000E-20
    NH4N            0 1.500E+00 1.000E+00 1.000E-20
    NH4S            0 1.500E+00 1.000E+00 1.000E-20
    SOA             4 1.000E+00 5.000E-01 1.000E-20
    POA             4 1.000E+00 2.000E-01 1.000E-20
    SOA1            4 1.000E+00 5.000E-01 1.000E-20
    SOA2            4 1.000E+00 5.000E-01 1.000E-20
    SOA3            4 1.000E+00 5.000E-01 1.000E-20
    SOA4            4 1.000E+00 5.000E-01 1.000E-20
    PEC             5 1.000E+00 2.000E-01 1.000E-20
    PMFINE          6 1.000E+00 2.000E-01 1.000E-20
    PMCOARS         7 1.000E+00 2.000E-01 1.000E-20
 reaction parameters record
     Rate const  Phot  Temp  Pres    #     Act Energy
  1    1.000E+00    T     F     F     0          0.0
  2    4.323E+06    F     T     F     1     -11750.0
  3    2.664E+01    F     T     F     2      13700.0
     ...
     ...
     ...
 75    9.924E+04    F     T     F     2      -4490.0
 76    1.100E-01    F     T     F     2       8210.0
```

```
  77    9.820E+03     F    T     F     2      -1750.0
 entered rvmmap
    8 fine grids defined.
 the following definition of fine grids
 will be used:


    horizontal subdivisions:

    00000000000000000000000000000000000000000000000000000000000000000000000
    0000000000000000000000
     ...
     ...
     ...
    00000000000000000000000000000000000000000000000000000000000000000000000
    0000000000000000000000

    map of grid id nos.:

    00000000000000000000000000000000000000000000000000000000000000000000000
    0000000000000000000000
     ...
     ...
     ...
    00000000000000000000000000000000000000000000000000000000000000000000000
    0000000000000000000000
 no file opened for wind for fine grid  1
     ...
 no file opened for wind for fine grid  8
 no file opened for kv for fine grid  1
     ...
 no file opened for kv for fine grid  8
 no file opened for pressure for fine grid  1
     ...
 no file opened for pressure for fine grid  8
 no file opened for ozone for fine grid  1
     ...
 no file opened for ozone for fine grid  8
 open unit 90 file /m2/remsadow/big_run/extra/sfc1.gis
 for surface char. for fine grid  1
     ...
 open unit 97 file /m2/remsadow/big_run/extra/sfc8.gis
 for surface char. for fine grid  8
 open unit 41 file
/m2/remsadow/eps2/omef_all/emiss.all.base96.pm.jan.wkd.3hrblk.r1.a0
 for weekday emissions for fine grid  1
 open unit 71 file
/m2/remsadow/eps2/omef_all/emiss.all.base96.pm.jan.sat.3hrblk.r1.a0
 for saturday emissions for fine grid  1
 open unit 72 file
/m2/remsadow/eps2/omef_all/emiss.all.base96.pm.jan.sun.3hrblk.r1.a0
 for sunday emissions for fine grid  1
     ...
     ...
     ...
 open unit 48 file
/m2/remsadow/eps2/omef_all/emiss.all.base96.pm.jan.wkd.3hrblk.r8.a0
```

```
 for weekday emissions for fine grid  8
 open unit 85 file
/m2/remsadow/eps2/omef_all/emiss.all.base96.pm.jan.sat.3hrblk.r8.a0
 for saturday emissions for fine grid  8
 open unit 86 file
/m2/remsadow/eps2/omef_all/emiss.all.base96.pm.jan.sun.3hrblk.r8.a0
 for sunday emissions for fine grid  8


    38326 point sources are involved in this simulation;  and source emissions=
T
 source number     1
 stack parameters
    -86.47    32.42    92.68    33.27    62.20    2.32    422.00    31.50
 source number     2
 stack parameters
    -86.47    32.42    92.68    33.27    57.90    1.22    350.00    6.00
 source number     3
 stack parameters
    -86.47    32.42    92.68    33.27    59.40    0.61    486.00    35.00
 source number     4
 stack parameters
    -86.47    32.42    92.68    33.27    76.20    1.52    466.00    7.00
 source number     5
 stack parameters
    -86.47    32.42    92.68    33.27    76.20    4.57    471.00    10.40
 in setup nopts =      38326
 total area and point source emissions (moles/min)
 area   0.3412E+06   0.0000E+00   0.0000E+00   0.3305E+05   0.8741E+05
0.1160E+07   0.0000E+00   0.0000E+00
   0.2233E+07   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   0.1525E+06
0.0000E+00   0.8665E+05
   0.2713E+06   0.6596E+01   0.1856E+02   0.0000E+00   0.0000E+00   0.0000E+00
0.2670E+06   0.2247E+07
   0.6105E+06   0.3187E+07   0.1260E+08
point   0.2810E+06   0.0000E+00   0.0000E+00   0.3116E+05   0.6826E+04
0.9055E+05   0.0000E+00   0.0000E+00
   0.3470E+06   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   0.4552E+06
0.0000E+00   0.0000E+00
   0.2031E+05   0.2314E+01   0.3044E+02   0.0000E+00   0.0000E+00   0.0000E+00
0.2552E+05   0.2172E+06
   0.9531E+05   0.6374E+06   0.9919E+06
Emission totals for fine grid     1
 TFAREA=
  1.8512E+03  0.0000E+00  0.0000E+00  8.4862E+01  4.5091E+02  5.9813E+03
0.0000E+00  0.0000E+00  7.7025E+03  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  1.2770E+02  0.0000E+00  1.1657E+02
     ...
     ...
     ...
Emission totals for fine grid     8
 TFAREA=
  2.1832E+03  0.0000E+00  0.0000E+00  2.2368E+02  6.7475E+02  8.9504E+03
0.0000E+00  0.0000E+00  2.4275E+04  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  1.0027E+03  0.0000E+00  4.1508E+03
 closed ic file (unit  24)
 no file opened for deposition velocities...
```

4

```
 dry deposition will be calculated internally.
 open unit=28  file=/m2/remsadow/big_run/extra/bndry.remsad.bin
for boundary concentrations

 Boundary definition for 104 rows
(***,***)( 21,125)( 20,125)( 20,125)( 20,125)( 20,125)( 19,126)( 19,126)( 19,126)(
19,126)
( 19,126)( 18,126)( 18,127)( 18,127)( 18,127)( 17,127)( 17,127)( 17,127)( 17,128)(
17,128)
( 16,128)( 16,128)( 16,128)( 16,128)( 15,129)( 15,129)( 15,129)( 15,129)( 15,129)(
14,129)
( 14,130)( 14,130)( 14,130)( 13,130)( 13,130)( 13,130)( 13,131)( 13,131)( 12,131)(
12,131)
( 12,131)( 12,131)( 11,132)( 11,132)( 11,132)( 11,132)( 11,132)( 10,132)( 10,133)(
10,133)
( 10,133)(  9,133)(  9,133)(  9,133)(  9,134)(  9,134)(  8,134)(  8,134)(  8,134)(
8,134)
(  7,135)(  7,135)(  7,135)(  7,135)(  7,135)(  6,135)(  6,136)(  6,136)(  6,136)(
5,136)
(  5,136)(  5,136)(  5,137)(  5,137)(  4,137)(  4,137)(  4,137)(  4,137)(  3,138)(
3,138)
(  3,138)(  3,138)(  3,138)(  2,138)(  2,139)(  2,139)(  2,139)(  1,139)(  1,139)(
1,139)
(  1,140)(
1,140)(***,***)(***,***)(***,***)(***,***)(***,***)(***,***)(***,***)(***,***)
(***,***)(***,***)(***,***)(***,***)(


 Boundary definition for 140 columns
(***,***)( 87, 93)( 83, 93)( 78, 93)( 74, 93)( 69, 93)( 65, 93)( 60, 93)( 56, 93)(
51, 93)
( 47, 93)( 42, 93)( 38, 93)( 33, 93)( 29, 93)( 24, 93)( 20, 93)( 15, 93)( 11, 93)(
6, 93)
(  2, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(
1, 93)
(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(
1, 93)
(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(
1, 93)
(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(
1, 93)
(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(
1, 93)
(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(
1, 93)
(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(
1, 93)
(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(
1, 93)
(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(
1, 93)
(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  1, 93)(
1, 93)
(  1, 93)(  1, 93)(  1, 93)(  1, 93)(  6, 93)( 12, 93)( 18, 93)( 24, 93)( 30, 93)(
36, 93)
( 42, 93)( 48, 93)( 54, 93)( 60, 93)( 66, 93)( 72, 93)( 78, 93)( 84, 93)( 90,
93)(***,***)
```

```
     WARNING: at source 14380 stkht=0.3000E+00 This is outside the internal check
range, but will be used
       ...
     WARNING: at source 38172 temps=0.1220E+03 This is outside the internal check
range, but will be used
       ...


                    Initial Concentrations      ◄──────────────────  5
Number of active cells: 10983


                         Minimum    Maximum     Average
 layer  1 NO             1.00E-11   1.00E-11    1.00E-11
     ...
     ...
     ...
 layer 15 PMCOARS        1.00E-07   1.00E-07    1.00E-07
     All variables read in setup lie within allowable limit

Time  100.   Date 980101
Updated input variables have the following ranges
Number of active cells: 10983


                         Minimum    ◄──────────  6  rage
                                     Maximum

 layer  1 u (m/s)        -1.38E+01   1.77E+01    1.62E+00
 layer  1 v (m/s)        -1.64E+01   1.52E+01   -2.87E-01
     ...
 layer 15 u (m/s)         1.05E+01   7.15E+01    3.11E+01
 layer 15 v (m/s)        -2.87E+01   3.28E+01   -1.90E+00
 layer  1 abs(u)          1.02E-03   1.77E+01    4.26E+00
 layer  1 abs(v)          5.68E-04   1.64E+01    4.94E+00
     ...
 layer 15 abs(u)          1.05E+01   7.15E+01    3.11E+01
 layer 15 abs(v)          1.93E-04   3.28E+01    1.04E+01
 layer  1 tot speed       7.13E-02   1.99E+01    7.14E+00
     ...
 layer  1 p (mb)          6.77E+02   1.03E+03    9.62E+02
     ...
 layer  1 z (m)           2.52E+01   3.18E+01    2.89E+01
     ...
 layer  1 kh (km2/min)    2.06E-03   5.48E+00    7.72E-01
     ...
 layer  1 kv (m2/s)       1.00E+00   1.26E+01    4.64E+00
     ...
 layer  1 temp (k)        2.40E+02   2.98E+02    2.75E+02
     ...
 layer  1 h2o (g/g)       6.81E-05   1.74E-02    4.47E-03
     ...
 layer  1 cloud cover     0.00E+00   1.00E+00    5.76E-03
     ...
 layer  1 ozone (ppm)     0.00E+00   0.00E+00    0.00E+00
     ...
 rain fall (in/hr)        0.66E-07   1.89E-01    8.63E-03
 dep vel (m/s)NO          0.00E+00   0.00E+00    0.00E+00
Number of boundary cells:  458
```

```
layer  1 bc NO           1.00E-11    1.00E-11    1.00E-11
     ...
     ...
layer 15 bc PMCOARS      1.00E-07    1.00E-07    1.00E-07


Mass flux summary in moles for fine grid  1 at     7  .00  980101:

Spec = NO           North                                       |
          In   0.000E+00              Srf emiss  0.000E+00 |
          Out  0.000E+00              Elv emiss  0.000E+00 |
          Net  0.000E+00              Depostn    0.000E+00 |
                                                           |
      West         Top         East                        |
In   0.000E+00   0.000E+00   0.000E+00                      |
Out  0.000E+00   0.000E+00   0.000E+00                      |
Net  0.000E+00   0.000E+00   0.000E+00                      |
                                                           |
                  South                                    |
          In   0.000E+00                                   |
          Out  0.000E+00              Tot mass   2.656E-01 |
          Net  0.000E+00                                   |
                                                           |
-----------------------------------------------------------------
     ...
     ...
     ...
```

Table 5-1.
Structure of the coarse-grid AVERAGE file.

Header Records

(1) The *File Description Header Record* contains 76 words:

1−10	A	File name = 'AVERAGE'; 10 characters, one character per word.
11−70	A	File identifier; 60 characters, one character per word.
71	I	Number of segments; must be 1.
72	I	Number of chemical species.
73	I	Beginning date of the file (Julian).
74	R	Beginning time of the file (hours).
75	I	Ending date of the file (Julian).
76	R	Ending time of the file (hours).

Words 73−76 describe the total time span contained on the file.

(2) The *Region Description Header Record* contains 15 words; the first three define the reference origin:

1	R	x-coordinate (UTM units).
2	R	x-coordinate (UTM units).
3	I	UTM zone.

The next two words define the location of the modeling region with respect to the reference origin:

4	R	x-location (meters).
5	R	y-location (meters).

The next two words define the size of each grid cell:

6	R	Grid cell size in the x-direction (meters).
7	R	Grid cell size in the y-direction (meters).

The next three words define the size of the modeling region in terms of the number of grid cells:

8	I	Number of grid cells in the x-direction.
9	I	Number of grid cells in the y-direction.
10	I	Number of grid cells in the z-direction.

The last five words describe the vertical distribution of grid cells (**not used in ATDM**):

11	I	Number of cells between the surface layer and diffusion break.
12	R	Number of cells between the diffusion break and top of region.
13	R	Height of surface layer (m).
14	R	Minimum cell height between surface layer and diffusion break.
15	R	Minimum cell height between diffusion break and top of region.

(3) The *Segment Description Header Record* contains one group of four words for the one segment (the number of segments is 1 in the File Description Header Record):

1	I	x-location of the segment origin with respect to origin of modeling region (grid units).
2	I	y-location of the segment origin with respect to origin of modeling region (grid units).
3	I	Number of grid cells in the segment, x-direction.
4	I	Number of grid cells in the segment, y-direction.

(4) The *Species Description Header Record* contains 10 words for each species (the number of species is defined in the File Description Header Record):

1-10	A	Species name; 10 characters, one character per word.

Time-Invariant Data

The AVERAGE file contains no time-invariant data.

Time-Varying Data

The AVERAGE file contains one set of the following records for each time interval.

(1) The *Time Interval Record* contains four words:

1	I	Beginning date (Julian).
2	R	Beginning time (hours).
3	I	Ending date (Julian).
4	R	Ending time (hours).

(2) There is a set of *Average Concentration Records* for the one segment of the region for each species,

ordered within each species by vertical layer. The first 11 words of the record identify segment and species:

      1   I   Segment number (must be 1).

     2–11   A   Species name; 10 characters, one character per word.

     The next series of words is the concentration array itself:

     12+   R   Concentrations ($\mu g/m^3$)averaged over the time interval for each cell in one vertical level. Values are ordered by x and y location of the cells as follows: ((C(I,J),I=1,NX),J=1,NY)

Table 5-2.
Format of the nested -grid AVERAGE concentration file (binary).

Record No.	Variables	Data type	Description
1	MSG	Character*80	Text identifying the simulation.
2	NUMFIN, NAVSPC	Integer, integer	Number of fine grids and number of species on file.
3	(MAVSPC(N), N=1,NAVSPC)	Character*10	Names of species, stored as 10 character strings.
4 (This record is included NUMFIN times, once for each fine grid.)	IXFB, JYFB, IXFE, JYFE, NHF, NVF, NFX, NFY, NFZ, IFGPTR, IFGLVL	All integer	IXFB, IXFE—first and last x cell of coarse grid subdivided for this fine grid.
			JYFB, JYFE—first and last y cell of coarse grid subdivided for this fine grid.
			NHF, NVF—number of fine grid cells per coarse grid cell horizontally and vertically.
			NFX, NFY—number of cells in x and y direction in fine grid.
			NFZ—number of layers in fine grid (regardless of the value of NFZ, only layer 1 is written to the output file).
			IFGPTR—points to fine-grid number in which this grid is nested (if 0, then this grid is only within the coarse grid).
			IFGLVL—depth at which this grid is nested (1 means within coarse grid only, 2 is within one other fine grid, 3 is within a fine grid which is within another fine grid, and so forth).
The following records are included at each model output time (usually hourly):			
5	TIME, NDATE	Real, integer	TIME is a real number representing military time (e.g., 2300. = 11:00 PM). NDATE is an integer representing the date either as a calendar date (YYMMDD) or a Julian style date (YYDDD). The concentrations that follow are averaged over the output interval with the time and data specifying the ending time of the averaging interval.
Repeat enclosed group of records for each fine grid (NUMFIN times)			
Repeat record 6 for each species (NAVSPC times)			
6	((AVCONF(I,J), I=1,NFX), J=1,NFY)	Real	Predicted concentrations ($\mu g/m^3$) in each cell of layer 1 of the fine grid.

Table 5-3.
Structure of the coarse-grid DEPOSITION file.

Header Records

(1) The *File Description Header Record* contains 76 words:

1−10	A	File name = 'DEPOSITION'; 10 characters, one character per word.
11−70	A	File identifier; 60 characters, one character per word.
71	I	Number of segments; must be 1.
72	I	Number of chemical species.
73	I	Beginning date of the file (Julian).
74	R	Beginning time of the file (hours).
75	I	Ending date of the file (Julian).
76	R	Ending time of the file (hours).

Words 73−76 describe the total time span contained on the file.

(2) The *Region Description Header Record* contains 15 words; the first three define the reference origin:

1	R	x-coordinate (UTM units).
2	R	x-coordinate (UTM units).
3	I	UTM zone.

The next two words define the location of the modeling region with respect to the reference origin:

4	R	x-location (meters).
5	R	y-location (meters).

The next two words define the size of each grid cell:

6	R	Grid cell size in the x-direction (meters).
7	R	Grid cell size in the y-direction (meters).

The next three words define the size of the modeling region in terms of the number of grid cells:

8	I	Number of grid cells in the x-direction.
9	I	Number of grid cells in the y-direction.
10	I	Number of grid cells in the z-direction.

The last five words describe the vertical distribution of grid cells (**not used in ATDM**):

11	I	Number of cells between the surface layer and diffusion break.
12	R	Number of cells between the diffusion break and top of region.
13	R	Height of surface layer (m).
14	R	Minimum cell height between surface layer and diffusion break.
15	R	Minimum cell height between diffusion break and top of region.

(3) The *Segment Description Header Record* contains one group of four words for the one segment (the number of segments is 1 in the File Description Header Record):

1	I	x-location of the segment origin with respect to origin of modeling region (grid units).
2	I	y-location of the segment origin with respect to origin of modeling region (grid units).
3	I	Number of grid cells in the segment, x-direction.
4	I	Number of grid cells in the segment, y-direction.

(4) The *Species Description Header Record* contains 10 words for each species (the number of species is defined in the File Description Header Record):

1-10	A	Species name; 10 characters, one character per word.

Time-Invariant Data

The DEPOSITION file contains no time-invariant data.

Time-Varying Data

The DEPOSITION file contains one set of the following records for each time interval.

(1) The *Time Interval Record* contains four words:

1	I	Beginning date (Julian).
2	R	Beginning time (hours).
3	I	Ending date (Julian).
4	R	Ending time (hours).

(2) There is a set of *Deposition Records* for the one segment of the region for each species, ordered within each

---

species by vertical layer. The first 11 words of the record identify segment and species:

1	I	Segment number (must be 1).
2–11	A	Species name; 10 characters, one character per word.

The next series of words is the array itself:

12	R	Dry deposition (g/km^2) over the time interval for each cell in layer 1. Values are ordered by x and y location of the cells as follows: ((C(I,J),I=1,NX),J=1,NY)
1	I	Segment number (must be 1).
2–11	A	Species name; 10 characters, one character per word.

The next series of words is the array itself:

13	R	Wet deposition (g/km^2) over the time interval for each cell in layer 1. Values are ordered by x and y location of the cells as follows: ((C(I,J),I=1,NX),J=1,NY)

Record 2 is repeated for each species (NAVSPE times)

Table 5-4.
Format of the nested -grid DEPOSITION file (binary).

Record No.	Variables	Data type	Description
1	MSG	Character*80	Text identifying the simulation.
2	NUMFIN, NAVSPC	Integer, integer	Number of fine grids and number of species on file.
3	(MAVSPC(N), N=1,NAVSPC)	Character*10	Names of species, stored as 10 character strings.
4 (This record is included NUMFIN times, once for each fine grid.)	IXFB, JYFB, IXFE, JYFE, NHF, NVF, NFX, NFY, NFZ, IFGPTR, IFGLVL	All integer	IXFB, IXFE—first and last x cell of coarse grid subdivided for this fine grid. JYFB, JYFE—first and last y cell of coarse grid subdivided for this fine grid. NHF, NVF—number of fine grid cells per coarse grid cell horizontally and vertically. NFX, NFY—number of cells in x and y direction in fine grid. NFZ—number of layers in fine grid (regardless of the value of NFZ, only layer 1 is written to the output file). IFGPTR—points to fine-grid number in which this grid is nested (if 0, then this grid is only within the coarse grid). IFGLVL—depth at which this grid is nested (1 means within coarse grid only, 2 is within one other fine grid, 3 is within a fine grid which is within another fine grid, and so forth).
The following records are included at each model output time (usually hourly):			
5	TIME, NDATE	Real, integer	TIME is a real number representing military time (e.g., 2300. = 11:00 PM). NDATE is an integer representing the date as a Julian style date (YYDDD). The concentrations that follow are over the output interval with the time and data specifying the ending time of the interval.
Repeat enclosed group of records for each fine grid (NUMFIN times)			
Repeat record 6 and 7 for each species (NAVSPC times)			
6	((DRYDEP(I,J), I=1,NFX), J=1,NFY)	Real	Predicted dry deposition (g/km^2) in each cell of layer 1 of the nested grid.
7	((WETDEP(I,J), I=1,NFX), J=1,NFY)	Real	Predicted wet deposition (g/km^2) in each cell of layer 1 of the nested grid.

Table 5-5
Structure of coarse-grid INSTANT file (binary).

Header Records

The INSTANT file contains observed concentration values as a function of time for each species over the region (x,y,z). The INSTANT file begins with the four standard header records.

(1) The *File Description Header Record* contains 76 words:

1–10	A	File name = 'INSTANT'; 10 characters, one character per word.
11–70	A	File identifier; 60 characters, one character per word.
71	I	Number of segments; must be 1.
72	I	Number of chemical species.
73	I	Beginning date of the file (Julian).
74	R	Beginning time of the file (hours).
75	I	Ending date of the file (Julian).
76	R	Ending time of the file (hours).

(2) The *Region Description Header Record* contains 15 words; the first three define the reference origin:

1	R	x-coordinate (UTM units).
2	R	y-coordinate (UTM units).
3	I	UTM zone.

The next two words define the modeling region location with respect to the reference origin:

4	R	x-location (meters).
5	R	y-location (meters).

The next two words define the size of each grid cell in the x- and y-direction.

6	R	Grid cell size, x-direction (meters).
7	R	Grid cell size, y-direction (meters).

The next three words define the size of the modeling region in grid cells.

8	I	Number of grid cells, x-direction.
9	I	Number of grid cells, y-direction.
10	I	Number of grid cells, z-direction.

The last five words describe the vertical distribution of grid cells (**not used in ATDM**).

11	I	Number of cells between surface layer and diffusion break.
12	I	Number of cells between diffusion break and top of region.
13	I	Height of surface layer (m).
14	R	Minimum cell height between surface layer and diffusion break (m).
15	R	Minimum cell height between diffusion break and top of region (m).

(3) The *Segment Description Header Record* contains four words for each segment (as specified in the File Description Header Record; for the UAM-V, only one segment is allowed):

1	I	x-location of segment origin with respect to origin of modeling region (grid units).
2	I	y-location of segment origin with respect to origin of modeling region (grid units).
3	I	Number of grid cells in segment, x-direction.
4	I	Number of grid cells in segment, y-direction.

(4) The *Species Description Header Record* contains 10 words for each species (the number of species is defined in the File Description Header Record):

1–10	A	Species name; 10 characters, one character per word.

Time-Invariant Data

The INSTANT file contains no time-invariant data.

Time-Varying Data

The INSTANT file contains one set of the following records for each time interval.

(1) The *Time Interval Record* contains four words:

1	I	Beginning date (Julian).
2	R	Beginning time (hours).
3	I	Ending date (Julian).
4	R	Ending time (hours).

(2) For the one segment of the region the INSTANT file contains a set of *Concentration Records* for each species, and ordered within each species by vertical level. The first 11 words of the record identify the

segment and species:

1	I	Segment number (must be 1).
2–11	A	Species name; 10 characters, one character per word.

The next series of words is the concentration array itself:

12+	R	Concentration (ppm) for each cell in one vertical level, varying by x-, then y-direction.

Table 5-6.
Format of the nested grid instantaneous concentration file (binary).

Record No.	Variables	Data type	Description
1	MSG	Character*80	Text identifying the simulation.
2	NUMFIN, NOSPEC	Integer, integer	Number of fine grids and number of species on file.
3	((MSPEC(I,N), I=1,10), N=1,NOSPEC)	Integer	Names of species, stored one character per integer word, 10 characters per name.
4 (This record is included NUMFIN times, once for each fine grid.)	IXFB, JYFB, IXFE, JYFE, NHF, NVF, NFX, NFY, NFZ, IFGPTR, IFGLVL	All integer	IXFB, IXFE—first and last x cell of coarse grid subdivided for this fine grid.
			JYFB, JYFE—first and last y cell of coarse grid subdivided for this fine grid.
			NHF, NVF—number of fine-grid cells per coarse-grid cell horizontally and vertically.
			NFX, NFY—number of cells in x and y direction in fine grid.
			NFZ—number of layers in fine grid.
			IFGPTR—points to fine-grid number in which this grid is nested (if 0, then this grid is only within the coarse grid).
			IFGLVL—depth at which this grid is nested (1 means within coarse grid only, 2 is within one other fine grid, 3 is within a fine grid which is within another fine grid, and so forth).

The following records are included at each model output time (usually hourly):

| 5 | TIME, NDATE | Real, integer | TIME is a real number representing military time (e.g., 2300. = 11:00 PM). NDATE is an integer representing the a Julian style date (YYDDD). The concentrations that follow are not averaged over time, but rather are concentrations predicted at this time and date. |

Repeat enclosed group of records for each nested grid (NUMFIN times)

    Repeat enclosed group of records for each species (NOSPEC times)

        Repeat record 6 for each layer (NFZ times)

| 6 | ((CNCF(I,J), I=1,NFX), J=1,NFY) | Real | Predicted concentrations (ppm) in each cell of one layer of the nested grid. |

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6. STANDARD REMSAD POSTPROCESSING PROCEDURES

For most REMSAD applications, graphical and statistical analysis will be used to review, analyze, and interpret the REMSAD modeling results. There are a variety of commercial software packages that facilitate the preparation of graphical displays and statistical summaries and we assume that the choice of graphical and statistical analysis software will vary among REMSAD users. Regardless of the display and analysis software, it is likely that users will first elect to extract a subset of species from the REMSAD AVERAGE output file, and calculate monthly, seasonal, and/or annual averages. Software for extracting and calculating specific averages and totals is provided as part of the REMSAD modeling system, and its application is described in this section of the users guide. The extraction software also accommodates the calculation of various visibility metrics, and the details of the visibility calculations are provided. This section concludes with some suggestions for statistical and graphical analysis.

The EXTRACT program accommodates standard manipulation of the REMSAD output files. The EXTRACT program reads the binary average concentration, instantaneous concentration, or deposition directly, and extracts the information specified by the user.

For ease of reading, all exhibits follow the text of this section.

6.1. EXTRACT Program

The EXTRACT module supports two types of extractions: horizontal cross sections (XYSEC), and visibility metrics (XYVIS). EXTRACT requires the user to set up an input file with information on the extraction selections. A single input file may be used to produce several extractions, or a separate input file may be created for each. If more than one extraction is performed with a single input file, a blank line (or comment line) should be inserted between each extraction. Input option files for each postprocessing module are in free format, with the exception of the input line in which the user specifies the name and units of measurement of the pollutant species to be extracted. The format for the EXTRACT option file is presented in Exhibit 6-1.

Maximum array dimensions and all global arrays for the EXTRACT program are contained in an "include" file. Array dimensions must be large enough to accommodate the modeling domain dimensions. Unless otherwise noted all references to REMSAD AVERAGE files will also apply to REMSAD instantaneous concentration (INSTANT) files and deposition files.

6.1.1. Input Requirements and Common or Typical Options

EXTRACT can produce extractions (or subset output files) for each of the REMSAD modeling grids separately, or for the entire grid (with an effective resolution of the finest nested grid). Several examples of EXTRACT input option files are given in Exhibits 6-1 through 6-10. Additional examples accompany the transmittal of the software.

In the EXTRACT input file, the type of extraction is first specified. Options are XYSEC or XYVIS. Each extraction requires, as input, an REMSAD binary coarse-grid average concentration file. A nested-grid average filename can also be provided (on a subsequent line or record); if none is given, the extraction will be performed on the coarse-grid file alone. Note that a single nested-

grid average file contains simulated concentrations for all nested grids included in the simulation. If a nested-grid filename is given, the user is then asked to enter the number of grids to be used in the extraction and the numbers of those nested grids. Grid number 0 refers to the coarse grid; fine grids are referred to by the number listed in the REMSAD diagnostic output or DIAG file (refer to Section 5). If nested-grids are included in the extraction, the resolution of the output will correspond to that for the finest grid specified (i.e., the output for coarser grids will be interpolated to this resolution). This change in resolution affects the number of grid cells in the extracted file. If a 12 km nested grid is extracted with a 36 km coarse grid, the resulting extracted file will include 3 times as many cells in the x and y directions as the coarse grid file did. The include file with maximum array dimensions (see previous section) must include dimensions large enough for the number of grid cells resulting in the extracted file.

The REMSAD boundary condition file (which also contains information about the modeling domain) may be provided to the EXTRACT program. If no boundary filename is specified, a boundary of one cell width around the perimeter of the modeling domain will be assumed. If no boundary file is deemed necessary, the user should specify the name of a dummy file (/dev/null) of zero length in the boundary filename input line.

Several user-specified options are common to the extraction types. The user specifies the number of pollutant species to be extracted from the file. The user may elect to convert the output values to a different unit of measurement than that used by REMSAD (e.g., ppb rather than ppm). The possibilities depend on the type of REMSAD output file being used. For AVERAGE and INSTANT files, the available units are ppm, ppb, micro-grams per cubic meter, nano-grams per cubic meter, pico-grams per cubic meter, and femto-grams per cubic meter. For DEPOSITION files the available units include grams per square kilometer, kilo-grams per square kilometer, micro-grams per square kilometer and kilo-grams per hectare.

Simulated values may be extracted from any vertical layer of the modeling domain by giving the number of layers for which data extraction is desired, and the number of each layer. This applies only to extractions from the REMSAD instantaneous concentration file, since the average file contains simulated concentrations for layer 1 only.

The user may define an extraction subdomain by entering SUB, followed by the grid cells of the southwest and northeast corners of the desired subdomain; otherwise, NOSUB may be entered and the entire domain will be used in the extraction. For a subdomain extraction, the grid cells specifying the southwest and northeast corners of the subregion must be given with respect to the domain origin of the input file(s) and the resolution of the output file.

The user also gives the starting and ending times and dates for each extraction; dates may be given in calendar (YYMMDD) or Julian (YYJJJ) format. The writing interval specifies the number of output intervals between extractions (e.g., an interval of 2 means data will be extracted for every other interval (e.g. odd numbered).

6.1.2. XYSEC Extraction

The XYSEC option is used to extract a horizontal cross section of simulated pollutant concentration or deposition from the REMSAD output files. Exhibits 7-1 through 7-9 depict various XYSEC extractions.

Several options may be used to specify what type of data file will be produced: MAP, MAX, AVE, DIF, MXDIF, SUM or TOT. The MAP option produces gridded predicted data of the specified pollutant for each extracted time interval specified by the user, while MAX produces

the maximum gridded concentrations or deposition within each grid cell over the course of the extraction interval. AVE provides the pollutant concentrations or deposition averaged over the extraction interval. If more than one averaging interval is desired, a separate input file should be created for each. The two DIF options are used to compare the output from two REMSAD simulations and, therefore, require two output files of the same type as input. If DIF or MXDIF is specified on the options input line, the second (or subtraction) filename should be entered on the line following this specification. Exhibit 6-6 is an example of a DIF extraction input file. DIF produces differences in the simulated values between the two files for each of the user-specified intervals, while MXDIF provides the difference in maximum concentrations at each grid cell over the entire extraction interval. In both cases the values in the second file listed in the EXTRACT input file are subtracted from those in the first.

The TOT option produces the summed total of concentration or deposition over the specified time interval for each grid cell.

The SUM option allows the user to define a composite species as a weighted sum of REMSAD modeled species. When the sum option is specified, the extraction will be formatted as for the MAP output. The resulting output file may then be input to EXTRACT again to perform other extraction types. Exhibits 6-4 and 6-7 illustrate this option.

In general, the output from an XYSEC extraction may be used as input to a subsequent XYSEC extraction. This allows the user to extract hourly data for a subset of the modeled species from the AVERAGE or INSTANT files and then use these output files to obtain daily maximums, daily averages, differences, etc.

When XYSEC extractions are performed for deposition, the user must specify some additional information concerning the type of deposition, as shown in Exhibits 6-4 and 6-5. The DEPOSITION files contain both wet and dry deposition predicted by the model. The user may specify to extract either dry deposition, wet deposition, or total (dry + wet) deposition.

Exhibit 6-9 illustrates an XYSEC extraction for subsequent use in calculating visibility measures. Note that all 11 species shown in the input file are required for the calculation of visibility measures and that the extraction can be performed only a single grid at a time.

6.1.3.   XYVIS Extraction

The XYVIS option is used to calculate visibility measures from the REMSAD modeled results. Three measures are calculated: extinction coefficient, visual range, and deciview. The resulting extraction (EXTRACT output) files contain gridded fields of these three visibility measures (for the time interval and each update interval specified).

The XYVIS option takes as input the extracted XYMAP file that contains all of the constituents needed for the calculation of the visibility measures (refer to Exhibits 6-9 and 6-10).

An example XYVIS extraction input file is provided by Exhibit 6-10. The first line is a comment line as in an XYSEC extraction, while the second line specifies XYVIS as the extraction type.

The following two lines specify the input and output filenames, respectively. Note that the input file must be the output from a previous XYSEC extraction and must contain all 11 species as shown in Exhibit 6-9.

The next three input lines specify the surface pressure, the temperature and the humidity data filenames. These files should be the same data files used in the REMSAD model run and must correspond to the particular grid used in the corresponding XYSEC extraction.

The next line specifies the number of grid cells in the x-, y-, and z-dimensions, as well as the grid cell size in the west-east and south-north directions.

The following input line specifies whether the grid is a [C]oarse or [F]ine grid data file. Note that currently only coarse grids may be specified for this type of extraction.

The remaining input lines specify the starting and ending time and date and the writing interval.

6.1.3.1.   Light Extinction

Atmospheric optical properties of air are characterized in terms of the ability of the gaseous and particulate constituents to absorb and scatter light. These properties are expressed as light absorption coefficient (b_{abs}), light scattering coefficient (b_{scat}), and their sum, light extinction coefficient (b_{ext}). These coefficients are formulated such that they represent cross-sectional area per unit volume of air; hence, their units are m^2/m^3 or m^{-1}. However, because the typical size of these coefficients is small the data are usually expressed in terms of μm^{-1} or $micron^{-1}$.

Generally, scattering is the more important of the two processes, as the concentration of particles available for effective scattering is generally much higher than that of particles available for effective absorption. Submicron particles between 0.1 to 1 μm are most effective at scattering visible light (with a wavelength between 0.4 and 0.7 μm) than are either smaller or larger particles. Table 6-1 shows the light extinction efficiency of common constituents of a polluted atmosphere. Light extinction coefficient (b_{ext}) is the product of the mass concentration and the light extinction coefficient efficiency of the given species as a function of wavelength.

Table 6-1.
Typical light extinction efficiencies for constituents of polluted atmospheres.

Constituent	Light Extinction Efficiency at $\lambda = 0.55$ μm (m^2/g)
Soot (elemental carbon)	13
Hygroscopic fine particulates including sulfates and nitrates	4–8
Fine Particles (0.1 to < 1μm)	3
Coarse Particles (1 to < 10 μm)	0.4
NO2	0.17
Giant Particles (> 10 μm)	< 0.04

Using the XYVIS extraction option, the REMSAD-derived extinction coefficient is determined by summing each species light extinction contribution. Extinction is reported for layer 1only and represents the mean value within the grid-cell.

6.1.3.2. *Deciview*

The deciview haze index (DV) has recently begun to be utilized as indicator of the clarity of the atmosphere that is more closely related to human perception (Pitchford and Malm, 1994). It is defined by the equation

$$DV = 10 \ln(\mathbf{b}_{ext}/10)$$

where b_{ext} is in μm^{-1}.

This index has value of approximately 0 when the extinction coefficient is equal to the scattering coefficient for particle-free air (Rayleigh scattering) and increases in value by approximately one unit for each 10 percent increase in b_{ext}. The apparent change in visibility is related to the percent change in b_{ext}, equal changes in DV correspond to approximately equal perceptible changes in visibility. A one DV change also has the interesting property of approximately corresponding to a human perceptible change in perception of a scene.

6.1.3.3. *Visual Range*

The visual, or meteorological, range is defined as the greatest distance at which a black target can be perceived against the horizon sky. In an idealized case, in which the atmosphere and its illumination are uniform for distances at least twice as great as the visual range, the assumption that a 2 percent contrast is just perceptible leads to the equation (Middleton, 1958).

$$rv = -\ln(0.02)/b_{ext} = 3.912/b_{ext}$$

This threshold contrast corresponds to viewing an object that subtends an angle of 3 to 6 minutes of arc in daytime. Note that small changes in b_{ext} have large effects on the visual range.

6.1.4. Extracting Tagging Information

Tagged species can be extracted and displayed in the same way that other species can. However, there are typically certain comparisons that are useful to make for the tagged species.

For a species such as cadmium, which does not have different chemical states to consider as does mercury, a useful initial extraction is a monthly average including all of the tagged cadmium species. (See the following section for specific procedures for accomplishing monthly averages.) For deposition, monthly total deposition files would be prepared. One of the cadmium tags normally includes emissions from all sources and also includes initial and boundary concentrations. This species would be extracted in the usual way in order to display simulated deposition or concentration of cadmium. Other tagged species can be extracted and displayed as if they were a standard species. For instance, if the CD-9 were used for initial and boundary concentrations, a display of deposition could be prepared showing the amount of background cadmium deposited. However, using the *filemath* routine, spatial plots can also be made of the percent contribution of a particular source type, or combination of source types. The display in Figure 6-1 shows the percent contribution of all Louisiana sources to cadmium deposition. The job that created the input file for the plot is presented in exhibit 6-11.

In the case of mercury, a step to sum the separate chemical species is usually desirable before processing the tagging information. If HG0-1, HG2-1, and HGP-1 are the mercury species corresponding to the different chemical forms of mercury that included all emissions and initial and boundary conditions, then a SUM would be run to prepare a THG species. This could be

done for either deposition or concentrations. Comparisons of the various tagged components can be made as described above for cadmium.

6.2. Calculation of Monthly, Seasonal, or Annual Averages and Deposition Totals

Daily averages and totals calculated using the EXTRACT program must be joined into longer (monthly, seasonal, or annual) files. This is done by the AVGJOIN program. AVGJOIN simply concatenates daily xymap files. Concatenated files must then be run through EXTRACT again to calculate averages or totals over the concatenated period. Please refer to Exhibit 6-12 for a sample AVGJOIN input stream.

6.3. Suggested Graphical Displays and Statistical Summaries

The following are some suggestions for display and analysis of REMSAD simulation results.

- Spatial distribution plots of simulated gaseous and particulate air constituents and deposition (an example spatial distribution for PM2.5 is provided in Figure 6-1).

    - Monthly, seasonal, and annual average values of ozone, NOx, CO, PM10, PM2.5, sulfate, nitrate, and ammonium.

    - Monthly, seasonal, and annual totals for sulfate, nitrate, ammonium, and mercury deposition (dry, wet, and total).

- Scatter plots comparing simulated and observed values of gaseous, particulate, and deposited species (an example scatter plot for mercury is given in Figure 6-2).

    - Seasonal and annual average PM10, PM2.5, sulfate, nitrate concentrations.

    - Seasonal and annual sulfate, nitrate, and mercury deposition (dry, wet, and total, depending upon data availability).

- Statistical measures such as normalized bias, normalized gross error, correlation, and root mean square error for all species with available data.

For REMSAD applications for the U.S., routine data sources include the EPA Aerometric Information Retrieval System (AIRS), the IMPROVE network, and the Mercury Deposition Network (MDN). Monitoring programs such as the SouthEast Aerosol Research and CHaracterization (SEARCH) study (sponsored by the Southern Company and the Electric Power and Research Institute) and Pacific 2001 (sponsored by Environment Canada) among other programs may provide more detailed information for the analysis of PM distribution and speciation.

Exhibit 6-1.
XYSEC MAP extraction input file: Nested grid extraction from INSTANT files.
Format of "SPECIES NAMES, UNITS" input line is A10,A8 (species name, units).

```
#### EXTRACT HOURLY O3 CONCS FROM INSTANT FILES
EXTRACTION TYPE      |XYSEC
AVERAGE FILENAME     |/a1/annual.pm/tmp/output/jul/INST/atdm.a_pm+tox.0701.inst
AVERAGE FILENAME     |/a1/annual.pm/tmp/output/jul/INST/atdm.a_pm+tox.0701.finst
# OF GRIDS           |3
GRID #'S             |0,1,2,3.
BOUNDARY FILENAME    |/a1/annual.pm/tmp/input/bndary.all.a2.bin
OUTPUT FILENAME      |/a1/annual.pm/tmp/postp/output/xymap.inst.cf.o3.0701.out
MAP,MAX,DIF,MAXDIF?  |MAP
# OF OUTPUT SPECIES  |1
SPECIES NAMES,UNITS  |O3        PPB
OF LAYERS, INDICES   |1,1
SUBDOMAIN            |NOSUB
STARTING TIME,DATE   | 1.            900701
ENDING TIME,DATE     | 1.            900702
WRITING INTERVAL     |1.
                     |
                     |
```

Exhibit 6-2.
XYSEC MAX extraction input file: Nested grid extraction from hourly (MAP) files.
Format of "SPECIES NAMES, UNITS" input line is A10,A8 (species name, units).

```
#### EXTRACT MAX O3 CONCS FROM HOURLY FILES
EXTRACTION TYPE      |XYSEC
AVERAGE FILENAME     |/a1/annual.pm/tmp/postp/output/xymap.cf.o3.0701.out
AVERAGE FILENAME     |
BOUNDARY FILENAME    |/dev/null
OUTPUT FILENAME      |/a1/annual.pm/tmp/postp/output/xymax.cf.o3.0701.out
MAP,MAX,DIF,MAXDIF?  |MAX
# OF OUTPUT SPECIES  |1
SPECIES NAMES,UNITS  |O3        PPB
OF LAYERS, INDICES   |1,1
SUBDOMAIN            |NOSUB
STARTING TIME,DATE   | 1.            900701
ENDING TIME,DATE     | 1.            900702
WRITING INTERVAL     |1.
                     |
                     |
```

Exhibit 6-3.
XYSEC MAP extraction input file:
Nested grid extraction from AVERAGE files with unit conversions.
Format of "SPECIES NAMES, UNITS" input line is A10,A8 (species name, units).

```
#### EXTRACT HOURLY O3 CONCS FROM AVERAGE FILES
EXTRACTION TYPE       |XYSEC
AVERAGE FILENAME      |/a1/annual.pm/tmp/output/jul/AVRG/atdm.a_pm+tox.0701.avrg
AVERAGE FILENAME      |/a1/annual.pm/tmp/output/jul/AVRG/atdm.a_pm+tox.0701.favrg
# OF GRIDS            |3
GRID #'S              |0,1,2,3.
BOUNDARY FILENAME     |/a1/annual.pm/tmp/input/bndary.all.a2.bin
OUTPUT FILENAME       |/a1/annual.pm/tmp/postp/output/xymap.cf.o3.0701.out
MAP,MAX,DIF,MAXDIF?   |MAP
# OF OUTPUT SPECIES   |1
SPECIES NAMES,UNITS   |O3        PPB
SURF PRESS FILENM     |/a1/annual.pm/tmp/mm4data/output/jul/0701-0710.crs.press
# LEVELS              |8
PTOP, SIGMA'S         |100.,0.98,0.93,0.84,0.7,0.5,0.3,0.1,0.0
TEMP FILNM            |/a1/annual.pm/tmp/mm4data/output/jul/0701-0710.crs.temp
OF LAYERS, INDICES    |1,1
SUBDOMAIN             |NOSUB
STARTING TIME,DATE    | 1.             900701
ENDING TIME,DATE      | 1.             900702
WRITING INTERVAL      |1.
                      |
                      |
```

Exhibit 6-4.
XYSEC extraction input file for depositions:
Nested grid composite (SUM)extraction for dry deposition of HGTOT.
Format of "SPECIES NAMES, UNITS" input line is A10,A8 (species name, units).

```
### EXTRACT HOURLY HG DEPOSITION FLUXES
EXTRACTION TYPE       |XYSEC
AVERAGE FILENAME      |/a1/annual.pm/tmp/output/jul/DEPN/atdm.a_pm+tox.0701.depn
AVERAGE FILENAME      |/a1/annual.pm/tmp/output/jul/DEPN/atdm.a_pm+tox.0701.fdepn
# OF GRIDS            |3
GRID #'S,TIME INCR    |0,1,2,3.
BOUNDARY FILENAME     |/a1/annual.pm/tmp/input/bndary.all.a2.bin
OUTPUT FILENAME       |/a1/annual.pm/tmp/postp/output/xymap.hgtot.ddep.cf.0701.out
MAP,MAX,DIF,MAXDIF?   |SUM
# OF OUTPUT SPECIES   |1
OUT SPEC NAME/UNIT    |HGTOT     G/KM2
# OF SPECIES IN SUM   |3
SPECIES NAME/FACTOR   |HG0       1.
SPECIES NAME/FACTOR   |HG2G      1.
SPECIES NAME/FACTOR   |HG2P      1.
WET, DRY, BOTH ?      |DRY
SUBDOMAIN             |NOSUB
STARTING TIME,DATE    | 1.             900701
ENDING TIME,DATE      | 1.             900702
WRITING INTERVAL      |1.
                      |
                      |
```

Exhibit 6-5.
XYSEC extraction input file for depositions:
Single nested grid extraction for dry deposition of HGTOT.
Format of "SPECIES NAMES, UNITS" input line is A10,A8 (species name, units).

```
#### EXTRACT HOURLY HG DEPOSITION FLUXES IN FINE GRID 1
EXTRACTION TYPE      |XYSEC
AVERAGE FILENAME     |/a1/annual.pm/tmp/output/jul/DEPN/atdm.a_pm+tox.0701.depn
AVERAGE FILENAME     |/a1/annual.pm/tmp/output/jul/DEPN/atdm.a_pm+tox.0701.fdepn
# OF GRIDS           |1
GRID #'S,TIME INCR   |1,3.
BOUNDARY FILENAME    |/a1/annual.pm/tmp/input/bndary.all.a2.bin
OUTPUT FILENAME      |/a1/annual.pm/tmp/postp/output/xymap.hgtot.ddep.f1.0701.out
MAP,MAX,DIF,MAXDIF?  |SUM
# OF OUTPUT SPECIES  |1
OUT SPEC NAME/UNIT   |HGTOT     G/KM2
# OF SPECIES IN SUM  |3
SPECIES NAME/FACTOR  |HG0       1.
SPECIES NAME/FACTOR  |HG2G      1.
SPECIES NAME/FACTOR  |HG2P      1.
WET, DRY, BOTH ?     |DRY
SUBDOMAIN            |NOSUB
STARTING TIME,DATE   | 1.             900701
ENDING TIME,DATE     | 1.             900702
WRITING INTERVAL     |1.
                     |
                     |
```

Exhibit 6-6.
XYSEC DIF extraction input file.

Format of "SPECIES NAMES, UNITS" input line is A10,A8 (species name, units).

```
#### XYDIF EXTRACT OF PMFINE FORM AVE EXTRACTION OUTPUT FILES
EXTRACTION TYPE      |XYSEC
AVERAGE FILENAME     |/a1/annual.pm/tmp/postp/output/xyave.cf.pmfine.0701.out
AVERAGE FILENAME     |
BOUNDARY FILENAME    |/dev/null
OUTPUT FILENAME      |/a1/annual.pm/tmp/postp/output/xydif.cf.pmfine.0701.out
MAP,MAX,DIF,MAXDIF?  |DIF
2nd AVERAGE FILE     |/a1/annual.pm/tmp/postp/output/xyave.cf.pmfine.0701.sns.out
# OF OUTPUT SPECIES  |1
SPECIES NAMES,UNITS  |O3        PPB
OF LAYERS, INDICES   |1,1
SUBDOMAIN            |NOSUB
STARTING TIME,DATE   | 1.             900701
ENDING TIME,DATE     | 1.             900702
WRITING INTERVAL     |1.
                     |
                     |
```

Exhibit 6-7.
XYSEC extraction input file for depositions:
Daily total (TOT) for dry deposition from hourly (MAP) files.

Format of "SPECIES NAMES, UNITS" input line is A10,A8 (species name, units).

```
### EXTRACT TOTAL HG DEPOSITION FLUXES
EXTRACTION TYPE      |XYSEC
AVERAGE FILENAME     |/a1/annual.pm/tmp/postp/output/xymap.hgtot.ddep.cf.0701.out
AVERAGE FILENAME     |
BOUNDARY FILENAME    |/a1/annual.pm/tmp/input/bndary.all.a2.bin
OUTPUT FILENAME      |/a1/annual.pm/tmp/postp/output/xytot.hgtot.ddep.cf.0701.out
MAP,MAX,DIF,MAXDIF?  |TOT
# OF OUTPUT SPECIES  |1
SPECIES NAMES,UNITS  |HGTOT     G/KM2
SUBDOMAIN            |NOSUB
STARTING TIME,DATE   | 1.            900701
ENDING TIME,DATE     | 1.            900702
WRITING INTERVAL     |1.
                     |
                     |
```

Exhibit 6-8.
XYSEC deposition extraction input file:
Subdomain extraction from daily total deposition file

Format of "SPECIES NAMES, UNITS" input line is A10,A8 (species name, units).

```
#### EXTRACT TOTAL DEPOSITION OF SPCNM[1] IN FINE GRID #l
EXTRACTION TYPE      |XYSEC
AVERAGE FILENAME     |/a1/annual.pm/tmp/postp/output/xytot.hgtot.ddep.cf.0701.out
AVERAGE FILENAME     |
BOUNDARY FILENAME    |/dev/null
OUTPUT FILENAME      |/a1/annual.pm/tmp/postp/output/xytot.hgtot.ddep.grd1.0701.out
MAP,MAX,DIF,MAXDIF?  |TOT
# OF OUTPUT SPECIES  |1
SPECIES NAMES,UNITS  |HGTOT     G/KM2
SUBDOMAIN            |SUB 144,102,190,157
STARTING TIME,DATE   | 1.            900701
ENDING TIME,DATE     | 1.            900702
WRITING INTERVAL     |1.
                     |
                     |
```

Exhibit 6-9.
XYSEC extraction input file for visibility species. All the species shown are required.

Format of "SPECIES NAMES, UNITS" input line is A10,A8 (species name, units).

```
#### EXTRACT SPECIES FOR VISIBILITY CALCULATIONS
EXTRACTION TYPE        |XYSEC
AVERAGE FILENAME       |/a1/annual.pm/tmp/output/jul/AVRG/atdm.a_pm+tox.0701.avrg
AVERAGE FILENAME       |
BOUNDARY FILENAME      |/a1/annual.pm/tmp/input/bndary.all.a2.bin
OUTPUT FILENAME        |/a1/annual.pm/tmp/postp/output/xymap.cc.vis.0701.out
MAP,MAX,DIF,MAXDIF?    |MAP
# OF OUTPUT SPECIES    |11
SPECS NAME/UNITS       |NO2       UG/M3
SPECS NAME/UNITS       |PNO3      UG/M3
SPECS NAME/UNITS       |GSO4      UG/M3
SPECS NAME/UNITS       |ASO4      UG/M3
SPECS NAME/UNITS       |NH4N      UG/M3
SPECS NAME/UNITS       |NH4S      UG/M3
SPECS NAME/UNITS       |SOA       UG/M3
SPECS NAME/UNITS       |POA       UG/M3
SPECS NAME/UNITS       |PEC       UG/M3
SPECS NAME/UNITS       |PMFINE    UG/M3
SPECS NAME/UNITS       |PMCOARS   UG/M3
OF LAYERS, INDICES     |1,1
SUBDOMAIN              |NOSUB
STARTING TIME,DATE     | 1.               900701
ENDING TIME,DATE       | 1.               900702
WRITING INTERVAL       |1.
                       |
                       |
```

Exhibit 6-10.
XYVIS extraction input file: Input AVERAGE file must be output
from extraction run shown in Exhibit 7-9 above.

```
#### CALCULATE AND EXTRACT VISBILITY MEASURES FOR COARSE GRID
EXTRACTION TYPE        |XYVIS
AVERAGE FILENAME       |/a1/annual.pm/tmp/postp/output/xymap.cc.vis.0701.out
OUTPUT FILENAME        |/a1/annual.pm/tmp/postp/output/xyvis.0701.out
PRESSURE FILENAME      |/a1/annual.pm/tmp/mm4data/output/jul/0701-0710.crs.press
TEMP FILENAME          |/a1/annual.pm/tmp/mm4data/output/jul/0701-0710.crs.temp
HUMIDITY FILENAME      |/a1/annual.pm/tmp/mm4data/output/jul/0701-0710.crs.humid
NX,NY,NZ,DX,DY         |90,56,8,0.66667,0.5
COARSE or FINE         |C
STARTING TIME,DATE     | 1.               900701
ENDING TIME,DATE       | 1.               900702
WRITING INTERVAL       |1.
                       |
                       |
```

Figure 6-10.
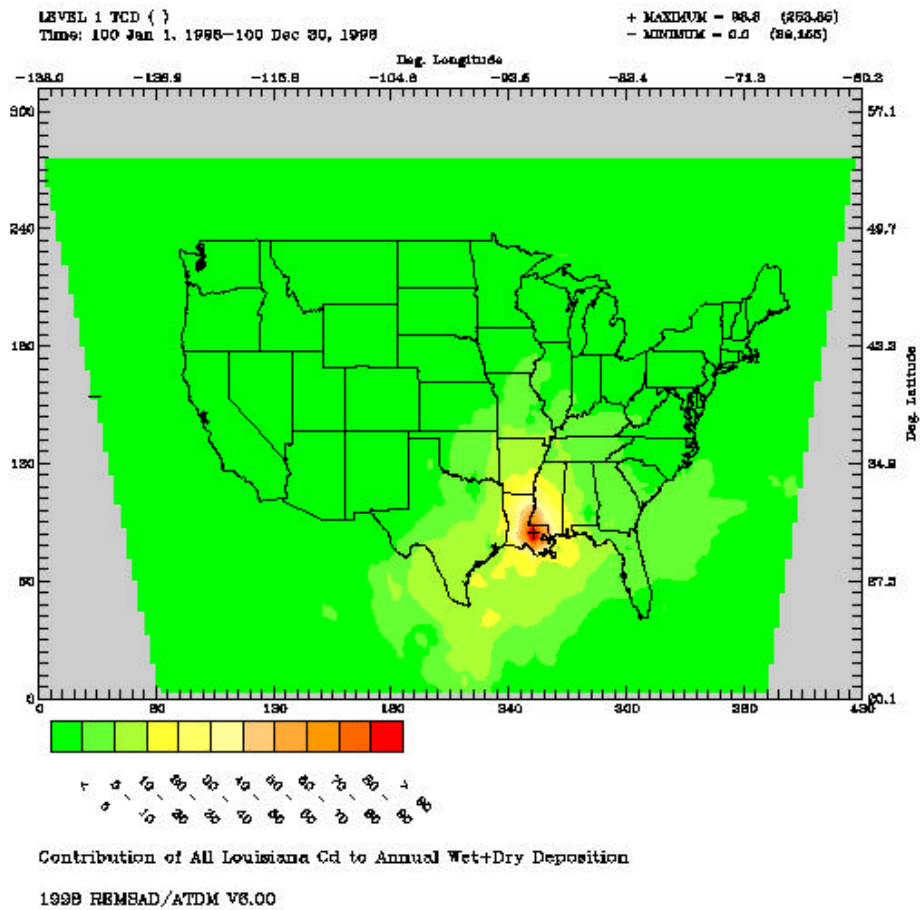**Percent Contribution of Louisiana Sources to Deposition.**

Exhibit 6-11.
FILEMATH job file to calculate percent contribution of Louisiana sources to deposition.

```
#!/bin/csh
set verbose
#
cd /a9/remsad96/big_run/postp/cadjobs
#
# calculate percent contribution of La. sources to deposition
#
setenv OUTDIR ../output/cdt/ANNUAL
#
# i=deposition
# j=scenario
#
set scen = (cdt.a0)
set dtyp = (wdep ddep dep)
#
foreach j (1)
foreach i (1 2 3)
#
rm $OUTDIR/xytot.$dtyp[$i].lapct.ann.$scen[$j].out
#
filemath << ieof
$OUTDIR/xytot.$dtyp[$i].lapct.ann.$scen[$j].out
FILE        $OUTDIR/xytot.$dtyp[$i].cd_5.ann.$scen[$j].out
FACTOR      100.
FILE        $OUTDIR/xytot.$dtyp[$i].cd_6.ann.$scen[$j].out
FACTOR      100.
FILE        $OUTDIR/xytot.$dtyp[$i].cd_7.ann.$scen[$j].out
FACTOR      100.
ADD
FILE        $OUTDIR/xytot.$dtyp[$i].cd_2.ann.$scen[$j].out
FILE        $OUTDIR/xytot.$dtyp[$i].cd_3.ann.$scen[$j].out
FILE        $OUTDIR/xytot.$dtyp[$i].cd_4.ann.$scen[$j].out
FILE        $OUTDIR/xytot.$dtyp[$i].cd_5.ann.$scen[$j].out
FILE        $OUTDIR/xytot.$dtyp[$i].cd_6.ann.$scen[$j].out
FILE        $OUTDIR/xytot.$dtyp[$i].cd_7.ann.$scen[$j].out
FILE        $OUTDIR/xytot.$dtyp[$i].cd_8.ann.$scen[$j].out
FILE        $OUTDIR/xytot.$dtyp[$i].cd_9.ann.$scen[$j].out
ADD
DIVIDE
ieof
#
end
end
```

Exhibit 6-12.
AVGJOIN input file: The "3" represents the number of individual files to join.
The final file is the output file.

```
1
3
/a1/annual.pm/tmp/postp/output/xyave.all.0101.crs.out
1
/a1/annual.pm/tmp/postp/output/xyave.all.0102.crs.out
1
/a1/annual.pm/tmp/postp/output/xyave.all.0103.crs.out
1
/a1/annual.pm/tmp/postp/output/xyave.all.jan.crs.out
```

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