USER'S GUIDE TO THE VARIABLE-GRID URBAN AIRSHED MODEL (UAM-V)

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Prepared by

Systems Applications International, Inc.

a subsidiary of ICF Consulting

101 Lucas Valley Road

San Rafael, California 94903

415/507-7100

ICF CONSULTING

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(This manual covers operation of UAM-V version 1.30.)

Contents

Figures

Tables

Exhibits

1. INTRODUCTION

The Urban Airshed Model (UAM) program was originally developed by Systems Applications International (SAI) and has been maintained by SAI for over 25 years. Its roots extend back to the earliest attempts at photochemical air quality modeling in the early 1970s. Since that time, the model has undergone a nearly continuous process of application, comprehensive performance evaluation, update, extension, and improvement.

The variable-grid Urban Airshed Model (UAM-V) system is the most current operational version of the UAM model. It incorporates multiple two-way grid nesting, allowing regional-scale ozone and precursor pollutant transport and several urban areas to be treated within a single modeling domain. In addition, the UAM-V program allows variability in the number and spacing of vertical layers, specification of three-dimensional meteorological variables, and explicit treatment of subgrid-scale photochemical plumes (i.e., plume-in-grid treatment). The UAM software was completely rewritten in a modular form for the UAM-V version, and includes updated deposition, plume-rise, solar flux, and chemical kinetics modules.

SAI has also developed input preparation packages with technical features commensurate with the requirements of the UAM-V system. These include a prognostic meteorological model with four-dimensional data assimilation (Douglas et al., 1991; Myers et al., 1991a) and a complete gridded emission inventory preparation system (Morris, Myers, and Haney, 1990; SAI, 1992). The UAM-V Postprocessing System (UPS) has also been developed to examine model output and assess model performance (SAI, 1996).

Conceptual Overview of the Model

The UAM-V model is a three-dimensional photochemical 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 model is usually exercised over a 48- to 120-hour ozone episode period.

The major factors that affect ozone air quality include:

- The spatial and temporal distribution of emissions of NO_x and volatile organic compounds (VOC) (both anthropogenic and biogenic).
- The composition of the emitted VOC and NO_x.
- The spatial and temporal variations in the wind fields.
- The dynamics of the boundary layer, including stability and the level of mixing.
- The chemical reactions involving VOC, NO_x, and other important species.
- The diurnal variations of solar insolation and temperature.
- The loss of ozone and ozone precursors by dry and wet deposition.
- The ambient background of VOC, NO_x, and other species in, immediately upwind, and above the region of study.

The UAM-V model simulates these processes when it is used to calculate ozone concentrations. It can also be used to simulate carbon monoxide concentrations in an urban area, a simulation that involves no chemical reactions. 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 UAM-V program performs this four-step solution procedure during each advective (driving) time step. The maximum advective time step is a function of the grid size and the maximum wind velocity or horizontal diffusion coefficient. Chemistry and vertical diffusion are solved on fractions of the advective time step to keep their individual numerical schemes stable. A typical driving time step for coarse (10-20 km) grid spacing is 10-15 minutes, whereas time steps for fine grid spacing (1-2 km) are on the order of a few minutes.

Because the UAM-V model accounts for spatial and temporal variations as well as differences in the reactivity (speciation) of emissions, it is ideally suited for evaluating the effects of emission control scenarios on urban air quality. The evaluation starts by replicating a historical ozone episode to establish a base-case simulation. Model inputs are prepared from observed meteorological, emission, and air quality data for a particular day or days using prognostic meteorological modeling and/or diagnostic and interpolative modeling techniques. The model is then applied with these inputs and the results are evaluated to determine its performance. Once the model results have been evaluated and determined to perform within prescribed levels, the same meteorological inputs and a *projected* emission inventory can be used to simulate possible future emission scenarios.

History of the Development of the Model

The UAM model has been under continual development for over 25 years, involving more than 100 person-years of technical effort. It has been supported by many organizations; both public and private organizations have contributed to the effort of demonstrating the utility of the UAM model to investigate and address complex ozone air quality management issues.

The history and development of mathematical photochemical models, particularly the UAM, has been paced by advances along three fronts:

- The *scientific front*, governed by the scientific community's acceptance of a suitable formulation, of supporting algorithms that represent pertinent physical and chemical processes, and of measurement methods and databases that support parameter estimation and model performance evaluations.
- The *regulatory front*, governed by the relevance and practicality of the UAM model to evolving regulatory programs and by acceptance of decisionmakers.
- The *computing technology front*, governed by the availability of computers capable of large-scale numerical modeling, by the transportability of the UAM model to those systems and by its being relatively friendly to users.

Since 1969, when the UAM program was first conceived, substantial changes have occurred on all three fronts. Some of these changes were anticipated, some changes were completely outside the control of the developers even when they were anticipated, and some were not anticipated. The initial model development and evaluation phase, from 1969 through 1973, culminated with the judgment by the EPA and its peer reviewers that the UAM approach was feasible and practical. This led to further development and evaluation, documented in a series of

reports (Liu et al., 1976; Reynolds et al., 1976; Lamb, 1976; Jerskey and Seinfeld, 1975; Killus et al., 1984; Lamb et al., 1984; Jerskey et al., 1984).

The 1980 public version of the model contained the Carbon-Bond Mechanism II (CB-II). In light of technical advances and experience with many different applications of the UAM system, this version of the model was updated in 1988. The two main improvements were the incorporation of the Carbon Bond Mechanism IV (Gery et al., 1988) and the use of the Smolarkiewicz numerical integration scheme to solve the advection equation (Smolarkiewicz, 1983). This version of the UAM model was released to the public in June 1990 (Morris, Myers, and Haney, 1990).

Although the 1990 version of the UAM model is the most widely used and evaluated air quality simulation model in the world, the structure of the software is based on 1970-1980 computing architecture and does not take advantage of the speed of current and future computer systems. Thus, in 1989-1991 SAI embarked on a massive effort to rewrite the model. The UAM program was refined and enhanced through the update of computer code and inclusion of the new capabilities, algorithms, modules, and features. The result, the UAM-V modeling system, has the following additional features over the 1990 version.

1. **Structured modular computer code:** The code is written in modular form for ease of inclusion of new modules and to take advantage of modern computers.

2. **Vertical grid structure:** The vertical layer structure can be arbitrarily defined by the user and is no longer defined from the diffusion break (mixing height). This allows for higher-resolution vertical layers near the surface and better matching with output from prognostic meteorological models, which usually use a terrain-following coordinate system.

3. **Three-dimensional inputs:** Several meteorological variables that were considered spatially constant in the UAM CB-IV (i.e., in the METSCALARS input file) now vary temporally and spatially (e.g., temperature, water vapor, pressure, and photolysis rates). Furthermore, the horizontal diffusivities and vertical turbulent exchange coefficients are now required as input, usually calculated with output from a prognostic meteorological model.

4. **Variable-grid resolution for chemical kinetic calculations:** When conditions permit, the chemistry calculations can be performed on aggregated blocks of cells rather than individual cells to reduce computation time.

5. **Two-way nested grid:** Finer grids can be embedded in coarser grids for more detailed representation of advection/diffusion, chemistry, and emissions. Several levels of nesting can be accommodated.

6. **Update of the CB-IV chemical mechanism:** The Carbon Bond IV chemical mechanism has been updated. The XO_2-HO_2 reaction has been added along with new temperature effects for PAN reactions. In addition, aqueous-phase (cloud) chemistry has been added as an option.

7. **New dry deposition algorithm:** The dry deposition algorithm formulated by Wesely (1989) has been implemented in the UAM-V program. This algorithm is similar to that used by the Regional Acid Deposition Model (RADM).

8. **True Mass Balance:** Concentrations are advected and diffused in the model using units of mass per unit volume rather than volumetric units (parts per million). When a given amount of ppm of a pollutant moves to a grid cell that has a different temperature or

pressure, there is a different amount of mass within the grid cell for the same ppm (ideal gas law). Using mass per unit volume maintains true mass balance in the advection and diffusion.

9. **Plume-in-Grid (PiG):** Emissions from point sources can be treated by a subgrid-scale Lagrangian photochemical plume model. Pollutant mass is released from the subgrid-scale model to the grid model when the plume size is commensurate with a grid cell size.

10. **New Plume Rise Algorithm:** A new plume rise algorithm has been implemented based on the one in the Gaussian dispersion model TUPOS (Turner et al., 1986).

The most recent version of the UAM-V modeling system (version 1.30) maintains the structure of, and backwards compatibility with, the earlier versions of the UAM-V, but includes major additional features. These include:

11. **CB-IV-TOX Chemical Mechanism:** This mechanism is an extension of the CB-IV mechanism, and includes a more detailed treatment of aldehyde chemistry (e.g., acetaldehyde is treated explicitly), the ability to track primary and secondary aldehydes, treatment of selected toxic species, and other improvements.

12. **Standard or Fast Chemistry Solver:** With the selection of a user-input flag, the model will either employ the standard chemistry solver or the fast chemistry solver.

13. **Process Analysis and Integrated Reaction Rates:** With the selection of a user input flag, the model will save detailed information on each of the physical (e.g. deposition, transport, etc.) and chemical transformation processes in each grid cell at each time step, in addition to the final concentration. This diagnostic tool provides for the examination of the contribution of each of the processes on the calculated concentration in a particular cell or group of cells.

Input Data Required by the UAM-V Model

The UAM-V derived pollutant concentrations are calculated from the emissions, advection, and dispersion of precursors and the formation and deposition of pollutants within every grid cell of the modeling domain. To adequately replicate the full three-dimensional structure of the atmosphere during an ozone episode, the UAM-V program requires an hourly and day-specific database for input preparation. Several preprocessing steps to translate raw emissions, meteorological, air quality, and grid-specific data are required to develop final UAM-V input files. The new features of the UAM-V model necessitate the provision of more extensive input data compared to the earlier version. For those familiar with the input data requirements of the UAM model, a comparison of UAM and UAM-V input data files is presented in Table 1-1. The structure and required formats of the UAM-V input data files are described in Section 4.

Observed air quality data are used to evaluate model predictions. These data may also be used to estimate the initial concentrations and boundary conditions for ozone, NO_x, and volatile organic compounds (VOC). The UAM-V model is usually used to simulate a multiday episode, and the simulation is started during the early morning hours one to three days before the start of episode. Use of start-up days limits the influence of the initial concentrations (which are not well known) on the simulation of the primary episode days.

Cell Aggregation and Grid Nesting

Although cell aggregation and grid nesting are optional, the model requires a definition of the grid structure. If these options are not utilized, an input file must be generated to indicate that only one uniform grid is to be defined, with no chemical cell aggregation.

It may be desirable to reduce computation time by performing chemical calculations on aggregated blocks of cells rather than individual cells. An aggregation input mapping field specifies which cells are to be aggregated. Cell aggregation may be done horizontally or vertically, and may be constant or time-varying.

Table 1-1.
UAM and UAM-V input data files

Data type	UAM files	UAM-V files
Meteorological	WIND (x, y-components of winds) TEMPARTUR (surface temperature) METSCALARS (spatially invariant water vapor, pressure, vertical temperature gradients, NO2 - photolysis rate, exposure class) DIFFBREAK (height of the "diffusion break") REGIONTOP (height of top of the region)	WIND (x, y-components of winds) TEMPERATURE (3D array of temperature) H2O (3D array of water vapor) VDIFFUSION (3D array of vertical turbulent diffusivity coefficients) HEIGHT (3D arrays of layer heights and pressure) RAIN (2D array of rainfall rates, optional) CLOUD (3D arrays of cloud cover and cloud water content, optional)
Surface characteristics	TERRAIN (surface roughness and deposition factor)	SURFACE (gridded land use) TERRAIN (terrain heights)
Emissions	EMISSIONS (surface emissions) PTSOURCE (elevated source emissions)	EMISSIONS (surface emissions) PTSOURCE (elevated source emissions)
Initial and boundary concentrations	AIRQUALITY (initial concentrations) BOUNDARY (lateral boundary concentrations) TOPCONC (concentrations at the top of the region)	AIRQUALITY (initial concentrations) BOUNDARY (lateral boundary concentrations) TOPCONC (concentrations at the top of the region)
Chemical rates	CHEMPARAM (chemical reaction rates)	CHEMPARAM (chemical reaction rates) RATES (tables of photolysis reaction rates) ALBEDO/HAZE/OZCOL (gridded albedo, haze and ozone column data)
Control	SIMCONTROL (simulation control information)	CONTROL (simulation control information) AGGMAP (cell aggregation) PACONTROL (process analysis control information)

Horizontal and vertical grid nesting can be defined for multiple fine grids. The horizontal structure of the nested grids is specified in the input parameter file.

Layer Heights and Pressure

The UAM-V grid contains a fixed number of vertical layers whose thickness can vary in space or time. The heights above ground level of the layer interfaces, and the atmospheric pressure at layer midpoints, at each horizontal grid location must be specified hourly. These values are usually determined to be consistent with the grid structure used in a prognostic meteorological model that is used to provide the meteorological inputs to the UAM-V program.

Land-Use Type and Surface Albedo

The percent coverage of 11 coded land-use categories are specified at each horizontal grid location for use in the dry deposition calculations. Land-use categories are typically obtained by averaging raw data from a geographic information system for each grid cell.

Gridded surface albedo indices based on land-use categories are also required for each horizontal grid location. These indices, which cross-reference the albedo values used in the photolysis rate preprocessor, are used to locate the proper photochemical reaction rates (or *J*-values) for the internal calculation of photolysis rates.

Terrain

Gridded terrain heights above mean sea level are specified for the coarse grid domain. However, the values of terrain heights are not used in the current version of the model. Terrain influence is communicated to the UAM-V program through the meteorological inputs. The terrain file also includes the coordinates of coarse grid cell centers in latitude/longitude coordinates.

Wind Components

Horizontal wind components (u and v) must be specified hourly for one of two optional configurations: winds at each grid cell center, or winds staggered to horizontal grid cell interfaces. Winds 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.

Temperature

The temperature must be specified hourly at the center of each grid cell; air temperature at the surface must be specified for each grid cell in layer 1. 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.

Vertical Exchange Coefficients

The vertical turbulent exchange coefficients (or diffusivities) must be specified hourly at the top of each grid cell (i.e., at the layer interface of each grid cell). The vertical diffusivities are necessary for evaluation of the vertical portion of the subgrid exchange term in the advection/diffusion equation. These values are usually obtained from either a prognostic meteorological model or a preprocessor that utilizes gridded UAM-V input wind and temperature data.

Water Vapor

The concentration of water vapor must be specified hourly at the center of each grid cell. Water vapor concentration is necessary for evaluation of certain reaction rates within the chemistry module.

Cloud Cover and Liquid Water Concentration (Optional)

The fraction of the sky covered by cloud (i.e., opacity) may be specified hourly for each grid cell. Cloud cover fraction is used to attenuate the photolysis rates calculated internally in the UAM-V model from the photolysis rate preprocessor. If this optional file is not used, photolysis rates are calculated assuming clear skies.

The liquid water concentration (optional) may be specified hourly at the center of each grid cell. This input is retained for compatibility with versions of UAM-V including aqueous-phase chemistry. However, aqueous-phase chemistry is not implemented in version 1.30.

Rainfall Rates (Optional)

Rainfall rates may be specified hourly at each horizontal grid location. If wet deposition is selected, the model requires gridded hourly rainfall rates to calculate the net removal of gases and aerosols by rain scavenging through the depth of each model column.

Initial Concentrations

The initial concentration of each species must be specified at the center of each grid cell. Initial concentrations can be uniform across the domain or can vary spatially in three dimensions. Initial concentrations are generally obtained through specifying constant values across the domain, or interpolation of observations. Use of one or more start-up days minimizes the effects of the initial concentration field on the episode days of interest.

Boundary Concentrations

The concentration of each species must be specified hourly at the center of each cell along the lateral boundaries and across the top of the modeling domain. Boundary conditions can be uniform or can vary spatially and temporally. Boundary conditions are required for evaluation of the advective transport term at grid cells adjacent to lateral boundaries when the relevant wind component is directed into the domain.

Boundary conditions aloft are required for the calculation of concentration in the top layer due to changes (spatial or temporal) in layer heights and depths (entrainment and dilution processes) or when vertical velocities are directed downward through the top of the domain. The vertical diffusion process does not affect concentrations aloft, due to specification of zero diffusive flux at the top of the domain.

Boundary conditions are generally obtained from preprocessors that can specify uniform or variant fields.

Area Source Emissions

The category of area sources includes true area sources (e.g., home heaters, dry cleaners, and solvent sources), mobile sources, low-level point sources (those with low stack heights or low effective plume rise), and biogenic and natural sources. Area source emission rates must be specified for each emitted species at each horizontal grid location; they can be optionally specified for each of 24 hours. Area source emissions are released into the first layer above the ground.

Elevated Point Source Emissions

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 of 24 hours. This file also identifies which point sources will be treated with the optional PiG treatment, with either full or simple chemical mechanisms.

Chemistry Parameters

A file containing the species to be simulated and various chemical reaction variables must be supplied to the UAM-V program for each application. Reaction variables include gas- and aqueous-phase reaction rates and activation energies. The chemical reaction variables should not be altered for individual applications; rather, they are only changed during upgrades to the chemical mechanism.

Photolysis Rates

The UAM-V program requires a multidimensional look-up table containing the photolysis rates (*J*-values) for seven chemical species. All other photolysis rates are calculated internally through application of scaling factors to the rates for these five species.

J-values are given for multiple solar zenith angles, altitudes, surface albedos, turbidity, and ozone column densities. The UAM-V program calculates day- and location-specific photolysis rates internally by (1) selecting the proper look-up table based on the input albedo, turbidity, and ozone column values; (2) estimating the solar zenith angle for the grid cell in question; and (3) locating in the selected look-up table the *J*-value corresponding to the local solar zenith angle and altitude.

Turbidity and Ozone Column

Indices that cross-reference turbidity and ozone column densities used in the photolysis rate preprocessor must be specified for each horizontal grid location. Like surface albedo, these indices are used to locate the proper *J*-value look-up table for the internal calculation of photolysis rates. Gridded data are obtained from a turbidity/ozone column preprocessor.

Aerosol Mass Distribution (Optional)

For aerosol species (e.g., sulfate), an aerosol mass distribution over eight bins is automatically set when the model is initialized. The number and range of each aerosol size bin are also set. Mass distributions are used for the calculation of particle dry deposition rates. Currently these mass distributions are only used for calculations involving sulfates. It is recommended that prior to using this feature, the user consult with the model developer.

Process Analysis and Integrated Reaction Rates (Optional)

When trying to gain insight into the most effective control strategy, or otherwise trying to diagnose or interpret model results, it is important to distinguish the processes that contribute to a resultant pollutant concentration. The process analysis extensions save additional information on the individual simulated effects of advection, diffusion, deposition, emissions, and chemistry, on chosen grid areas. In addition, the integrated reaction rates extensions save detailed information on the importance of each reaction within the chemical mechanism. The information saved can be analyzed to further evaluate and examine the contributions from each of the physical and chemical processes in a particular cell or group of cells.

Model Output

The UAM-V model provides gridded hour-averaged and instantaneous concentration output for all species and grids simulated. Separate concentration output files are created for the outer (or coarse) grid and for the nested grids. The hour-averaged concentrations are intended for comparison with measurements and ambient standards. The instantaneous concentration output is primarily used to restart the model. For restart purposes, PiG restart files are generated when the PiG treatment is in use. An optional PiG dump file can record PiG data for later use in preparing boundary concentrations for sub-domains.

An optional high-frequency ozone output file records surface ozone concentrations at intervals shorter than 1 hour. When using the process analysis technique, output files are generated that include data on concentration changes due to individual model processes.

Several runtime diagnostic files are also output. These contain information about computer resources required during the run, diagnostics on the various numerical schemes (as selected by the user), diagnostics on input data and selected internally calculated values (e.g., deposition velocity and PiG variables), and extensive mass budget calculations. These files will also display any runtime error or warning messages accrued.

2. TECHNICAL FORMULATION

The variable-grid Urban Airshed Model (UAM-V) system is a three-dimensional grid (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 basis for the UAM-V 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:

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

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

where

c_i	=	concentration of pollutant *i*, a function of space (*x,y,z*) and time (*t*)
u,v,w	=	horizontal and vertical wind speed 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

The model employs finite-difference numerical techniques for the solution of the advection/diffusion equation. The region to be simulated is divided into several three-dimensional grids covering the region of interest. A base coarse grid covering the entire domain must first be defined; then finer nested grids within the coarse grid may be defined for regions in which more refined analyses are desired. The model accepts nesting in both the horizontal and vertical, allowing for many levels of nesting if desired.

The vertical layer structure of the UAM-V model can be defined arbitrarily by the user. Usually, the vertical layers are defined to match the vertical layer structure of the meteorological model used to generate the UAM-V meteorological inputs (note that unlike previous versions of the UAM model, the vertical structure is not dependent on the mixing height). The UAM-V grid nesting in the vertical allows for the use of high resolution in regions where it is needed. For example, five vertical layers could be specified to resolve synoptic-scale transport and any other important features (e.g., a nocturnal jet) in the outer coarse grid region and 8–12 vertical layers could be defined in the innermost fine grid where high vertical resolution is needed to resolve complex transport features due to topographic or ocean/lake breeze effects.

The following subsections briefly describe each of the major processes of the UAM program. References are provided for a more detailed description of the treatments of the chemical and advection/diffusion processes.

Atmospheric Chemistry

Gas-Phase Chemistry

Ozone is formed in the atmosphere through chemical reactions between nitrogen oxides (NO_x) and volatile organic compounds (VOC). Hundreds of organic compounds and thousands of reactions participate in the formation of ozone in the atmosphere. The explicit treatment of all of these compounds and reactions would be prohibitively complex in a Eulerian-based grid model such as the UAM program. Thus most photochemical chemical kinetic mechanisms treat organic compounds in groups, often on the basis of the reactive functional groups they contain.

The UAM-V program employs an extension of version IV of the Carbon Bond Mechanism (CB-IV) for solving chemical kinetics (Gery et al., 1988). This extension called CB-IV-TOX expands the treatment of olefins and aldehydes including an explicit treatment of acetaldehyde. The carbon-bond approach disaggregates organic species based on the carbon bonds of the organic compounds. For example, propylene, butene, and 1-pentene each have one terminal olefinic carbon double bond but the number of single carbon bonds are different. Thus, in the carbon-bond approach propylene, butene, and 1-pentene would each be represented by one olefinic bond (OLE) and one, two, and three paraffinic bonds (PAR), respectively.

As implemented here, the CB-IV-TOX contains over 100 reactions and over 30 chemical species. The reactions are given in Table 2-1. Table 2-2 lists the species treated by the mechanism; representative values for the rates of seven photolysis reactions are given in Table 2-3. The UAM-V model contains significant updates to the CB-IV mechanism suggested by Dodge (1989) and others: an update to the PAN temperature effects (reactions 46–48), inclusion of a radical–radical reaction that acts as a radical sink under low NO_x concentration conditions (reaction 86), and revised isoprene chemistry based on Carter (1996).

The CB-IV-TOX was originally developed to enable more detailed study of aldehydes and their role in the formation of Polycyclic Organic Matter (POM) and has been used in several studies for urban scale modeling (Guthrie et al., 1997; Ligocki et al., 1992; Ligocki and Whitten, 1992; Ligocki et al., 1991a; Ligocki et al., 1991b). The CB-IV-TOX treats acetaldehyde explicitly instead of as ALD2. Standard CB-IV uses acetaldehyde chemistry as a surrogate for internal olefins and all aldehydes other than formaldehyde. In addition to acetaldehyde, CB-IV-TOX expands ALD2 to three species (ALDX for aldehydes with more carbons than acetaldehyde, IOLE for internal olefins, and PANX for C3 and greater PAN-like compounds). When originally expanded the “Tox” version produced essentially the same results as the regular CB-IV mechanism. However, it was subsequently realized that higher aldehydes apparently photolyze to free radicals as much as four times faster than acetaldehyde. This implies that the use of acetaldehyde as a surrogate for the higher aldehydes may underestimate the radical input from urban mixtures that have significant quantities of higher aldehydes and precursors to such aldehydes. Tests have shown the CB-IV-TOX to give as much as 30 percent more ozone at low VOC-to-NOx ratios compared to the standard CB-IV (which uses acetaldehyde photolysis for all aldehydes other than formaldehyde). Also, two smog chamber tests (one in Australia (Hess et al., 1992) and the other at TVA (Simonaitis et al., 1997)) have concluded that the standard CB-IV underpredicts ozone for urban mixtures (containing higher aldehydes or their precursors) at low VOC-to-NOx ratios.

However, at this point neither the Australian nor the TVA data have been simulated to verify this "fix."

The combination of the CB-IV-TOX treatment of aldehydes with the updated isoprene and radical chemistry make the CB-IV-TOX the most up to date and scientifically accurate version of the Carbon Bond Mechanism ever released.

The differential equations that describe the CB-IV are a "stiff" system; that is, the equations contain wide variations in time (reaction rate) constants. Solving these equations with a conventional numerical integrator for "stiff" systems, such as the one developed by Gear (1971), would result in prohibitively expensive computer time. Thus, the time integration of the CB-IV in the UAM model utilizes quasi-steady-state assumptions for species with large formation/removal rates (the "steady state species") and uses the computationally efficient Newton-Raphson algorithm for these steady state species. A Crank-Nicholson solution method is used for the remainder of the species (the "state species").

The development and formulation of the CB-IV mechanism is described in more detail by Gery et al. (1988, 1989). The numerical implementation of CB-IV in the UAM model is discussed more fully by Morris et al. (1990c,d).

Table 2-1.
The Carbon Bond Mechanism, Version IV-TOX, used in the UAM-V model, version 1.30

	Reaction		Rate Constant[a] @ 298 K (ppm^{-n} min^{-1})	E/R (K)
1	NO2	→ NO + O	Radiation Dependent[b]	
2	O	→ O3	4,323,000	-1175
3	O3 + NO	→ NO2	26.64	1370
4	O + NO2	→ NO	13,750	0
5	O + NO2	→ NO3	2309	-687
6	O + NO	→ NO2	2438	-602
7	NO2 + O3	→ NO3	0.04731	2450
8	O3	→ O	$0.053 \times k_1$	
9	O3	→ O1D	Radiation Dependent[b]	
10	O1D	→ O	424,600	-390
11	O1D + H2O	→ 2 OH	3.26	0
12	O3 + OH	→ HO2	100	940
13	O3 + HO2	→ OH	3	580
14	NO3	→ 0.89 NO2 + 0.89 O + 0.11 NO	$33.9 \times k_1$	
15	NO3 + NO	→ 2 NO2	44,160	-250
16	NO3 + NO2	→ NO + NO2	0.5901	1230
17	NO3 + NO2	→ N2O5	1853	-256
18	N2O5 + H2O	→ 2 HNO3	1.9×10^{-6}	0
19	N2O5	→ NO3 + NO2	2.776	10,900
20	NO + NO	→ 2 NO2	0.00015	-530
21	NO + NO2 + H2O	→ 2 HONO	3.0×10^{-8}	-6348
22	NO + OH	→ HONO	9799	-806
23	HONO	→ NO + OH	$0.1975 \times k_1$	
24	HONO + OH	→ NO2	9770	0
25	HONO + HONO	→ NO + NO2	0.00002	0
26	NO2 + OH	→ HNO3	16,820	-713
27	HNO3 + OH	→ NO3	217.9	-1000
28	NO + HO2	→ OH + NO2	12,270	-240
29	NO2 + HO2	→ PNA	2025	-749
30	PNA	→ HO2 + NO2	5.115	10,121
31	PNA + OH	→ NO2	6833	-380

	Reaction			Rate Constant[a] @ 298 K (ppm^{-n} min^{-1})	E/R (K)
32	HO2 + HO2	→	H2O2	4144	-1150
33	HO2 + HO2 + H2O	→	H2O2	0.2181	-5800
34	H2O2	→	2 OH	$0.255 \times k_{39}$	
35	H2O2 + OH	→	HO2	2520	187
36	CO + OH	→	HO2	322	0
37	FORM + OH	→	HO2 + CO	16,300	110
38	FORM	→	2 HO2 + CO	Radiation Dependent[b]	
39	FORM	→	CO	Radiation Dependent[b]	
40	FORM + O	→	OH + HO2 + CO	237	1550
41	FORM + NO3	→	HNO3 + HO2 + CO	0.93	0
42	ACET + O	→	C2O3 + OH	636	986
43	ACET + OH	→	C2O3	21,900	-205
44	ACET + NO3	→	C2O3 + HNO3	4.03	1860
45	ACET	→	FORM + 2 HO2 + CO + XO2	Radiation Dependent[b]	
46	C2O3 + NO	→	FORM + NO2 + HO2 + XO2	28,200	180
47	C2O3 + NO2	→	PAN	13,700	-380
48	PAN	→	C2O3 + NO2	0.0254	13,500
49	C2O3 + C2O3	→	2 FORM + 2 XO2 + 2 HO2	24,500	-530
50	C2O3 + HO2	→	0.33 O3	20,900	-1040
51	CH4 + OH	→	FORM + XO2 + HO2	10.34	1710
52	PAR + OH	→	0.87 XO2 + 0.13 XO2N + 0.11 HO2 + 0.06 ACET - 0.11 PAR + 0.76 ROR + 0.05 ALDX	1203	0
53	ROR	→	0.96 XO2 + 0.6 ACET + 0.94 HO2 2.1 PAR + 0.04 XO2N + 0.02 ROR + 0.5 ALDX	137,100	8000
54	ROR	→	HO2	95,445	0
55	ROR + NO2	→	NTR	22,000	0
56	OLE + O	→	0.24 ACET + 0.38 HO2 + 0.28 XO2 + 0.3 CO + 0.2 FORM + 0.02 XO2N + 0.22 PAR + 0.2 OH + 0.39 ALDX	5920	324
57	OLE + OH	→	FORM + 0.38 ACET +0.62 ALDX - PAR + XO2 + HO2	42,000	-504
58	OLE + O3	→	0.19 ACET + 0.31 ALDX + 0.74 FORM + 0.22 XO2 + 0.1 OH + 0.33 CO + 0.44 HO2 - PAR	0.018	2105

	Reaction	Rate Constant[a] @ 298 K (ppm^{-n} min^{-1})	E/R (K)
59	OLE + NO3 → 0.91 XO2 + FORM + 0.09 XO2N + 0.35 ACET + 0.56 ALDX + NO2 - PAR	11.35	0
60	ETH + O → FORM + 1.7 HO2 + CO + 0.7 XO2 + 0.3 OH	1080	792
61	ETH + OH → XO2 + 1.56 FORM + 0.22 ALDX + HO2	11,920	-411
62	ETH + O3 → FORM + 0.42 CO + 0.12 HO2	0.0027	2633
63	TOL + OH → 0.44 HO2 + 0.08 XO2 + 0.36 CRES + 0.56 TO2	9150	-322
64	TO2 + NO → 0.9 XO2 + 0.9 HO2 + 0.9 OPEN +NO + 0.1 XO2N	12,000	0
65	TO2 → CRES + HO2	250	0
66	CRES + OH → 0.4 CRO + 0.6 XO2 + 0.6 HO2 + 0.3 OPEN	61,000	0
67	CRES + NO3 → CRO + HNO3	32,500	0
68	CRO + NO2 → NPHN	20,000	0
69	OPEN → C2O3 + HO2 + CO	$9.04 \times k_{38}$	
70	OPEN + OH → XO2 + 2 CO + 2 HO2 + C2O3 + FORM	44,000	0
71	OPEN + O3 → 0.03 ALDX + 0.62 C2O3 + 0.7 FORM + 0.03 XO2 + 0.69 CO + 0.08 OH + 0.76 HO2 + 0.2 MGLY	0.015	500
72	XYL + OH → 0.7 HO2 + 0.5 XO2 + 0.2 CRES + 0.8 MGLY + 1.1 PAR + 0.3 TO2	36,200	-116
73	MGLY + OH → XO2 + C2O3	26,000	0
74	MGLY → C2O3 + HO2 + CO	$0.022 \times k_1$	
75	ISOP + O → 0.75 ISPD + 0.50 FORM + 0.25 X02 + 0.25 HO2 + 0.25 CXO3 + 0.25 PAR	53,200	0
76	ISOP + OH → 0.912 ISPD + 0.629 FORM + 0.991 XO2 + 0.912 HO2 + 0.088 X02N	147,600	-407.6
77	ISOP + O3 → 0.65 ISPD + 0.60 FORM + 0.20 X02 + 0.066 HO2 + 0.266 OH + 0.20 CXO3 + 0.15 ALDX + 0.35 PAR + 0.066 CO	0.019	1912
78	ISOP + NO3 → 0.20 ISPD + 1.0 X02 + 0.80 HO2 + 0.20 NO2 + 0.80 ALDX + 2.4 PAR + 0.8 NTR	996	448
79	XO2 + NO → NO2	12,000	0
80	XO2 + XO2 →	2000	-1300
81	XO2N + NO → NTR	12,000	0
82	ETOH + OH → HO2 + 0.95 ACET + 0.78 FORM + 0.05 XO2 + 0.011 ALDX	4840	66.8
83	ETOH + NO3 → HO2 + ACET + HNO3	1.33	0
84	MEOH + OH → FORM + HO2	1375	0
85	MEOH + NO3 → HO2 + FORM + HNO3	0.33	0

	Reaction		Rate Constant[a] @ 298 K (ppm^{-n} min^{-1})	E/R (K)
86	XO2 + HO2	→	8,900	-1300
87	XO2N + HO2	→	8,900	-1300
88	XO2N + XO2N	→	2,000	-1300
89	XO2N + XO2	→	4,000	-1300
90	ALDX + O	→ CXO3 + OH - PAR	632.	986.
91	ALDX + OH	→ CXO3 - PAR	24000.	-250.
92	ALDX NO3	→ CXO3 + HNO3 - PAR	4.03	1860.
93	ALDX	→ ACET + 2.0 HO2 + CO + XO2 - PAR	Radiation Dependent[b]	
94	IOLE + O	→ 1.14 ACET + 0.76 ALDX + 0.1 HO2 + 0.1 XO2 + 0.1 CO + 0.1 PAR	34000.	0.
95	IOLE + OH	→ 1.2 ACET + 0.8 ALDX + HO2 + XO2	94300.	-550.
96	IOLE + O3	→ 0.60 ACET + 0.40 ALDX + 0.25 FORM + 0.25 CO + 0.5 O + 0.5 OH + 0.5 HO2	0.31	1100.
97	IOLE + NO3	→ 1.09 ACET + 0.73 ALDX + HO2 + NO2	573.	270.
98	CXO3 + NO	→ ACET + NO2 + HO2 + XO2	28200.	180.
99	CXO3 + NO2	→ PANX	13700.	-380.
100	PANX	→ CXO3 + NO2	2.54E-2	13500.
101	CXO3 + C2O3	→ ACET + FORM + 2.0 XO2 + 2.0 HO2	24500.	-530.
102	CXO3 + HO2	→ 0.33 O3	20900.	-1040.
103	PANX + OH	→ ACET + NO2	1700.	0.
104	OH + HO2	→	1.626E5	-250.
105	ISPD + OH	→ 1.565 PAR + 0.167 FORM + 0.713 XO2 + 0.503 HO2 + 0.334 CO + 0.168 MGLY + 0.253 ACET + 0.21 C2O3 + 0.288 CXO3 + 0.021 ALDX	49.660	0
106	ISPD + O3	→ 0.114 C2O3 + 0.15 FORM + 0.85 MGLY + 0.154 HO2 + 0.268 OH + 0.064 XO2 + 0.02 ACET + 0.36 PAR + 0.225 CO	0.0105	0
107	ISPD + NO3	→ 0.357 ALDX + 0.282 FORM + 1.282 PAR + 0.925 HO2 + 0.643 CO + 0.075 CXO3 + 0.075 XO2 + 0.075 HNO3 + 0.85 NTR	1.478	0
108	ISPD	→ 0.333 CO + 0.067 ACET + 0.90 FORM + 0.832 PAR + 1.033 HO2 + 0.70 XO2 + 0.967 C2O3 + 0.7 CXO3	Radiation dependent[b]	
109	ISOP + NO2	→ 0.20 ISPD + 1.0 XO2 + 0.80 HO2 + 0.20 NO + 0.80 ALD2 + 2.4 PAR + 0.8 NTR	0.00022	0

	Reaction			Rate Constant[a] @ 298 K (ppm^{-n} min^{-1})	E/R (K)
110	MTBE + OH	→	1.37 XO2 + 0.98 HO2 + 0.42 FORM + 0.97 PAR + 0.02 XO2N	4100.	0
111	SO2 + OH	→	SULF + HO2	1110	-160
112	SO2	→	SULF	8.167E-5	0

[a] Pressure dependent values for the concentrations of M and O_2 are included in the rate constants where appropriate: [M] = 10^6 ppm, [O_2] = 2.095×10^5 ppm.

[b] Representative values for the rates of photolysis reactions 1, 9, 38, 39, 45, 93, and 108 are given in Table 2-3.

[c] In the UAM-V, the concentration of methane is assumed to be spatially invariant and therefore [CH_4] of 1.85 ppm is included in the rate constant for reaction 51.

Table 2-2.
Chemical species in the CBM-IV

Species Name	Representation
Nitric oxide	NO
Nitrogen dioxide	NO2
Nitrate radical	NO3
Dinitrogen pentoxide	N2O5
Nitrous acid	HONO
Nitric acid	HNO3
Peroxynitric acid (HO_2NO_2)	PNA
Oxygen atom (singlet)	O1D
Oxygen atom (triplet)	O
Hydroxyl radical	OH
Water	H2O
Ozone	O3
Hydroperoxy radical	HO2
Hydrogen peroxide	H2O2
Carbon monoxide	CO
Formaldehyde (HCHO)	FORM
Acetaldehyde	ACET
High molecular weight aldehydes (RCHO, R>H2)	ALDX
Internal olefins	IOLE
Peroxyacyl radical ($CH_3C(O)OO\cdot$)	C203
C3 and higher peroxy radicals	CXO3
Peroxyacyl nitrate ($CH_3C(O)OONO_2$)	PAN
C3 and higher PAN-like compounds	PANX
Nitrophenol	NPHN
Paraffin carbon bond (C-C)	PAR
Secondary organic oxy radical	ROR
Olefinic carbon bond (C=C)	OLE
Ethene ($CH_2=CH_2$)	ETH
Toluene ($C_6H_5-CH_3$)	TOL
Cresol and higher molecular weight phenols	CRES
Toluene-hydroxyl radical adduct	TO2
Methylphenoxy radical	CRO
High molecular weight aromatic oxidation ring fragment	OPEN
Xylene ($C_6H_4-(CH_3)_2$)	XYL
Methylglyoxal ($CH_3C(O)C(O)H$)	MGLY
Isoprene	ISOP
Organic residue after isoprene reaction	ISPD
Methanol	MEOH
Ethanol	ETOH
Methyl-tertiarybutylether	MTBE
Sulfur dioxide	SO2
Sulfate	SULF
NO-to-NO_2 operation	XO2
NO-to-nitrate operation	XO2N
Organic-nitrate	NTR

Table 2-3.
Representative values for the photolysis rates for reactions 1, 9, 38, 39, 45, 108, and 93 (J_{NO2}, J_{O1D}, J_{HCHOr}, J_{HCHOs}, J_{ACETr}, $J_{Acrolein}$, J_{ALDX} respectively) from the UAM-V

Solar Zenith Angle	Photolysis Rate (min^{-1})						
	J_{NO2}	J_{O1D}	J_{HCHOr}	J_{HCHOs}	J_{ACETr}	$J_{Acrolein}$†	J_{ALDX}
0	5.699×10^{-1}	2.595×10^{-3}	2.129×10^{-3}	2.848×10^{-3}	3.909×10^{-4}	1.117×10^{-4}	1.346×10^{-3}
10	5.654×10^{-1}	2.507×10^{-3}	2.097×10^{-3}	2.816×10^{-3}	3.820×10^{-4}	1.106×10^{-4}	1.319×10^{-3}
20	5.516×10^{-1}	2.252×10^{-3}	1.999×10^{-3}	2.721×10^{-3}	3.558×10^{-4}	1.072×10^{-4}	1.239×10^{-3}
30	5.276×10^{-1}	1.860×10^{-3}	1.834×10^{-3}	2.556×10^{-3}	3.136×10^{-4}	1.014×10^{-4}	1.109×10^{-3}
40	4.913×10^{-1}	1.380×10^{-3}	1.601×10^{-3}	2.314×10^{-3}	2.575×10^{-4}	9.276×10^{-5}	9.324×10^{-4}
50	4.393×10^{-1}	8.798×10^{-4}	1.299×10^{-3}	1.981×10^{-3}	1.912×10^{-4}	8.070×10^{-5}	7.184×10^{-4}
60	3.654×10^{-1}	4.418×10^{-4}	9.335×10^{-4}	1.540×10^{-3}	1.211×10^{-4}	6.432×10^{-5}	4.813×10^{-4}
70	2.597×10^{-1}	1.477×10^{-4}	5.278×10^{-4}	9.798×10^{-4}	5.711×10^{-5}	4.262×10^{-5}	2.480×10^{-4}
78	1.476×10^{-1}	3.856×10^{-5}	2.248×10^{-4}	4.806×10^{-4}	2.010×10^{-5}	2.209×10^{-5}	9.675×10^{-5}
86	4.393×10^{-2}	4.694×10^{-6}	3.916×10^{-5}	1.062×10^{-4}	2.806×10^{-6}	5.541×10^{-6}	1.546×10^{-5}

* Values are calculated for an altitude of 640 m above mean sea level, an ozone column of 300 Dobson units, a surface albedo of 0.05, and an optical depth due to absorption and scattering by atmospheric aerosols of 0.2.

† Used in estimating ISPD photolysis rate.

Photolysis Rates

Photochemical models require information on solar radiation in order to calculate photolysis rates for the photochemical reactions that drive the formation of ozone. The CB-IV chemical mechanism implemented in the UAM-V reads in photochemical reaction rates, or *J*-values, for seven processes: J_{NO2}, J_{O1D}, J_{HCHOr}, J_{HCHOs}, J_{ACETr}, J_{ALDX}, and $J_{Acrolein}$ (reactions 1, 9, 38, 39, 45, 93, and 108 in Table 2-1). Photolysis rates for several other photochemical reactions are derived from these *J*-values using scaling factors (see Gery et al., 1988).

The photolysis rate for a given process is expressed by the following integral:

$$J_n = \int_{\lambda_{min}}^{\lambda_{max}} I_n(\lambda) \bullet s_n(\lambda) \bullet f_n(\lambda)\, d\lambda$$

where $I(\lambda)$ is the wavelength-resolved actinic flux, $\sigma(\lambda)$ is the wavelength-resolved absorption cross-section for the species undergoing photolysis, and $\phi(\lambda)$ is the wavelength-resolved quantum yield for the photolysis process.

Evaluation of the above expression requires estimates of $\sigma(\lambda)$ and $\phi(\lambda)$. Data on $\sigma(\lambda)$ can be obtained from the following sources:

NO_2	DeMore et al., 1983
HCHO	Cantrell et al., 1990; Rogers, 1990
O_3	Molina and Molina, 1986
ACETr	Baulch et al., 1984
ALDX	Atkinson et al., 1997

Data on $\phi(\lambda)$ can be obtained from the following sources:

NO_2	Gardner et al., 1987
HCHOr	Calvert, 1980
HCHOs	Calvert, 1980
O_3	DeMore et al., 1990
ACETr	Baulch et al., 1984
ALDX	Atkinson et al., 1997

Actinic flux $I(\lambda)$ varies in space and time and must therefore be estimated by the UAM-V program. It is a function of the following variables:

1. The extraterrestrial solar flux—a parameterization of the brightness of the sun at the top of the atmosphere (Fröhlich and Werhli, 1983).
2. Surface UV albedo—the amount of UV radiation reflected from the earth's surface, which is land-use dependent.
3. Turbidity—the optical extinction due to scattering and absorption by aerosols.
4. Total O_3 column density over the modeling domain—in Dobson units, latitudinally and seasonally dependent.

The extraterrestrial solar flux is determined by the solar zenith angle, which the UAM-V calculates from the latitude, day-of-the-year, and time-of-day. UV albedo is determined using the UAM-V land-use characteristics input data. Turbidity and O_3 column density are specified separately.

The calculations of *J*-values during UAM-V integration are performed on a cell-by-cell basis using data from a look-up table generated by a UAM-V photolysis rate preprocessor. The preprocessor incorporates a parameterized light-model developed by Schippnick and Green (1982) that can treat total O_3 column density, surface albedo and turbidity as variable inputs; therefore the *J*-value look-up table can be extended as needed to cover the ranges of these parameters encountered in the modeling region. Cloud cover is not treated by the preprocessor but is

handled within the UAM-V, to be discussed below. Using wavelength-resolved absorption cross-section and quantum yield data for each photolysis reaction, the resulting look-up table contains photolysis rates for various solar zenith angles and altitudes as functions of solar flux, albedo, turbidity, and ozone column density.

For each time step during UAM-V integration, the relevant photolysis rates are determined as follows:

1. The solar zenith angle for the grid cell is calculated based on the latitude/longitude, time of day, and date.
2. The average altitude of the grid cell is taken as the height of the midpoint of the grid cell above ground.
3. The hourly-average cloud cover in tenths of total coverage, the daily-average ozone column index, daily-average turbidity index, and surface albedo index for the grid cell are taken from gridded inputs of all these variables.
4. Indices for ozone column, albedo, and turbidity are used to locate the appropriate *J*-value look-up table generated by the photolysis rate preprocessor. Photolysis rates for the grid cell are then calculated by linear interpolation between the nearest values of solar zenith angle and altitude in the look-up table.
5. These photolysis rates are then corrected for cloud cover greater than 70% based on factors used in RADM. (Adjustment factors used are as follows for 70%, 80%, 90%, and 100% cloud cover: 0.72, 0.68, 0.64, 0.59.)

The cloud cover scaling factors applied to the NO_2 photolysis rates vary from 1 for clear skies to 0.59 for completely overcast conditions. Attenuation factors for other *J*-values may be different, although there is no information on the attenuation of photolysis rates for chemicals other than NO_2. Thus, as a first approximation we assume that the cloud cover effects for all photolysis rates are the same as for NO_2.

Pollutant Transport

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 UAM-V model.

Advection in the UAM model is treated by specifying horizontal wind fields (i.e., u and v wind components in each grid cell) for each vertical layer and each nested grid. The vertical velocity in the UAM-V terrain-following coordinate system is then calculated from the conservation of mass equation.

The UAM-V model has relied primarily on prognostic meteorological model output to define wind fields, although the model has also been applied using wind fields generated with objective analysis techniques of upper-air and surface meteorological observations (Morris et al., 1991c). To date, the UAM-V has been applied using meteorological fields generated by MM5, MC2, SAIMM, SUMM, and the RAMS prognostic meteorological models.

The UAM-V program has been set up with an option to accept meteorological inputs on an Arakawa-C grid as well as the usual configuration of defining all meteorological variables at the grid cell centers. This option is recommended if UAM-V meteorological inputs are to be

generated from the output of a meteorological model using an Arakawa-C grid (e.g., CALRAMS). In an Arakawa-C configuration, temperature and pressure are defined in the grid cell centers whereas 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 UAM-V model to represent vertical transport.

The positive-definite advection scheme developed by Smolarkiewicz (1983) is used to represent horizontal advection in the UAM-V model. This scheme has been adapted to both the cell-centered grid and the Arakawa-C (staggered) grid options. In idealized tests, several other advection algorithms exhibit less numerical diffusion than the Smolarkiewicz algorithm but require significantly greater computation time (Chock, 1991). It remains to be seen whether, under representative real-world flow conditions, these other algorithms produce noticeably different solutions from those of the Smolarkiewicz algorithm.

Grid Nesting

The UAM-V model can provide two-way interactive nesting of fine grids within coarser grids in both the horizontal and the vertical. The fine grids must be nested completely within the coarse grid domain, the edges of the fine grid must correspond to a coarse grid cell edge, and, currently, the fine grids must be rectangular in shape (or trapezoidal if a latitude/longitude coordinate system is being used). The horizontal spacing of a fine grid may be any integral subdivision of the coarser grid within which it is embedded. There may be many fine grids within a coarse grid, and there can be several levels of nesting (i.e., finer grids embedded within an embedded fine grid); however, fine grids cannot overlap each other. This nested-grid approach has been tested to assure accuracy and mass consistency (Morris et al., 1991a,b, 1992a,b; Myers et al., 1991).

Gridded low-level emissions data files must be supplied separately for the coarse and fine grids. Land-use, wind and diffusivity data for the fine grids may optionally be specified separately or interpolated from coarse-grid inputs. Other input data, such as temperature and water vapor concentrations, are always interpolated to the fine grids from the coarse grid inputs.

The UAM-V species continuity equation using nested grids is solved as follows:

1. Emissions are injected into the coarse grid.
2. Transport/diffusion/deposition are integrated on the coarse grid for one coarse-grid advective (driving) time step.
3. For each fine grid:
    (a) If necessary, coarse-grid input data are interpolated to the fine grid.
    (b) A driving time step is defined for the fine grid that is an integral subdivision of the coarse-grid time step.
    (c) Emissions are injected.
    (d) Transport/diffusion/deposition are integrated.
    (e) Chemistry calculations are carried out.

(f) Steps (c), (d), and (e) are repeated until a time period equal to the coarse-grid time step is completed.

4. Chemistry calculations are performed in those coarse-grid cells not covered by a fine grid.

Turbulent Diffusion

Diffusion of pollutants in the UAM-V model is assumed to be proportional to the concentration gradient in space (i.e., "K-theory" or "first-order closure"). The proportionality factor is termed the eddy diffusivity coefficient (K_X, K_Y, and K_V in the advection/diffusion equation).

Horizontal diffusivities are calculated within the UAM-V program based on deformation characteristics of the horizontal wind (Smagorinsky, 1963). Scaling factors are applied to the deformation terms based on the square of grid cell resolution; maximum and minimum allowable horizontal diffusivities are specified by the user.

Vertical turbulent exchange coefficients may be diagnosed from the UAM-V wind and temperature fields, or directly interpolated from K_V fields estimated using a prognostic meteorological model.

Zero-flux conditions are specified on all lateral boundaries for horizontal diffusion, and for the top of the model for vertical diffusion. The lower boundary condition for vertical diffusion is specified as the dry deposition flux from layer 1 to the surface.

Surface Removal Processes

The UAM-V dry deposition algorithm is based on the scheme in the RADM model described by Wesely (1989). It is described briefly in the following paragraphs; for more complete descriptions, see Gray et al. (1991) and Scire (1991).

In the model the flux of pollutant material to the lower boundary (surface) (F_0) is expressed as concentration in the first model layer (C_i) times deposition velocity (V_d):

$$F_0 = -C_i V_d$$

The deposition velocity is estimated as an inverse sum of a series of resistances. For gaseous species this is expressed as follows:

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

where

R_a = aerodynamic resistance

R_b = boundary layer resistance

R_s = surface resistance

The deposition velocity of particulate species also depends on the size distribution and density of the particles in question. Large particles have a significant sedimentation velocity (V_{sed}) that acts in parallel to the other resistances. Very small particles behave in a manner similar to gases,

albeit they diffuse more slowly. The simplistic expression for the particle deposition velocity is as follows:

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

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 quasilaminar 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). 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).

Micrometeorological Submodule

The UAM-V program calculates the friction velocity and Monin-Obukhov length, needed for the aerodynamic resistance calculation, from gridded input wind and temperature, based on similarity theory. It is assumed that a constant flux surface layer exists from the surface to the midpoint height of layer 1, regardless of layer 1 thickness. Pressure, surface temperature, and layer 1 temperature are used to calculate a potential temperature gradient, which is then combined with layer 1 wind speed to determine stability. Following the formulation of Louis (1979), stability, layer 1 wind speed, and surface roughness are used to calculate the 10-m wind, friction velocity, and Monin-Obukhov length for each land-use category. Recognizing that roughness of a water surface depends on surface stress, water roughness is recalculated from friction velocity for use in calculating the three deposition resistances. Friction velocity over water is loaded into a special variable for use in over-water surface resistance calculations.

Subgrid-scale Variation in Land Use

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.

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. The deposition algorithm in the model identifies three vegetative states for each grid cell; (A) active unirrigated vegetation in unstressed conditions, or irrigated vegetation; (B) active unirrigated vegetation in stressed conditions; and (C) inactive vegetation.

In state A, stomatal resistance is parameterized in terms of a reference resistance (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. If a more detailed breakdown of the agricultural land-use category into crop type can be obtained, this new temperature correction allows for easy implementation of crop-dependent minimum, maximum and optimum temperatures for stomatal closing. Currently, default values for minimum, maximum and optimum temperatures of 0, 40, and 20◦C, respectively, are used.

In state B, which should correspond to minimum stomatal opening, stomatal resistance is arbitrarily set to a multiple of state A resistance. Currently this factor is set at 10; this may not be an appropriate multiplier and should be reconsidered when moisture stress information is eventually made available to the model. In state C, stomatal resistance is set to a very large value (10^4), essentially cutting off the deposition pathway for the particular land-use category. 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, only state A is considered.

Deposition to Water Surfaces

Deposition to water surfaces can be rapid for many soluble gases, but the expected enhancement in deposition velocities to water is not well represented by the Wesely (1989) algorithm. Therefore, a formulation for surface resistance over water based on the work of Slinn et al. (1978) is implemented in the UAM-V model, as suggested by Scire (1991). In liquid-phase resistance is given by

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

where H is the Henry's law coefficient, α_* 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:

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

Effects of Surface Moisture

The UAM-V deposition algorithm includes modifications to the surface resistances for dew- and rain-wetted surfaces (Wesely, 1989). The extent of dew is estimated by the program based on a relationship between relative humidity and wind speed.

Rainfall rates, if supplied, are used to determine the temporal and spatial extent of rain-wetted ground. The input file used for this purpose is the same as that used for calculating wet deposition (see below). In the absence of this file, the model only considers surface resistance modifications due to dew-wetted ground.

Wet Deposition

The UAM-V model contains an optional wet deposition algorithm that calculates the removal of aerosol and soluble gas species from the atmosphere during rain events. An input file containing hourly gridded rainfall rates, usually based on available observed data, is required for this option.

The wet deposition option is generally not used for ozone modeling, since rainfall is uncommon during ozone episodes.

Treatment of Plume Rise

The treatment of plume rise in the UAM-V program is based on the plume rise treatment developed for the Gaussian dispersion model TUPOS (Turner et al., 1986). Plume rise is calculated from stack parameters and gridded UAM-V meteorological inputs. The routine calculates stability-dependent plume rise based on either buoyancy or momentum flux for the layer containing the stack, whichever is larger. If plume rise exceeds the top of a layer, plume rise is recalculated based on the local stability of the next higher layer along with a residual buoyancy flux into that layer (momentum flux applies in the stack layer only). Once final plume rise is established, the results are modified by Froude-number–dependent stack tip downwash if wind speeds are higher than 2/3 stack exit velocity.

Neutral-unstable momentum 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).

Neutral-unstable buoyancy rise ΔH_{ub} is taken as the lesser of

$$\Delta H_{ub} = 30 \left(f / u \right)^{3/5} + z_b \qquad (1)$$

and

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

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 buoyancy 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:

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

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.

Stable momentum rise is taken as the lesser of ΔH_{um} and the quantity ΔH_{sm}:

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

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

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

and

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

where f_0 is stack tip buoyancy flux and f can be either f_0 or f_r, depending on the layer in question. 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):

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

$$f_r = f - 0.24 \frac{\partial q}{\partial z} \frac{f_0^{1/3}}{T} \left(z_t^{8/3} - z_b^{8/3}\right) \qquad (4)$$

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

The calculation of plume rise continues layer by layer using 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.

Subgrid-Scale Treatment of Point Source Plumes

The UAM-V program contains a "plume-in-grid" (PiG) module that allows plumes from individual sources to be represented as a series of discrete subgrid-scale Gaussian puffs. The PiG module is a descendant of the Reactive Plume Model (Morris et al., 1992c).

The PiG option is especially recommended for treatment of large elevated NO_x sources, as instantaneous dispersion of NO_x emissions within a grid cell containing substantial concentrations of VOC can exaggerate the contribution of the NO_x to ozone production in that cell.

The PiG treatment is schematically depicted in Figure 2-1. Each puff is initialized with up to 10 concentric elliptical "reactor cells." The number of initial cells is a user option. As the puffs travel within the model grid, they entrain "ambient" air from surrounding grid cells and undergo chemical transformations. Although each puff interacts with the grid cell in which it is located, puffs do not interact with each other. When the dimensions of a puff are commensurate with the dimensions of a grid cell, puff material from the outer cell is "shed" to the grid model. This process is repeated until the puff is eliminated.

Under unstable conditions a puff can grow very quickly in the vertical. To account for this growth, the entire mass of a puff is released to the cell containing the puff centerline if the puff volume exceeds one-half the grid-cell volume.

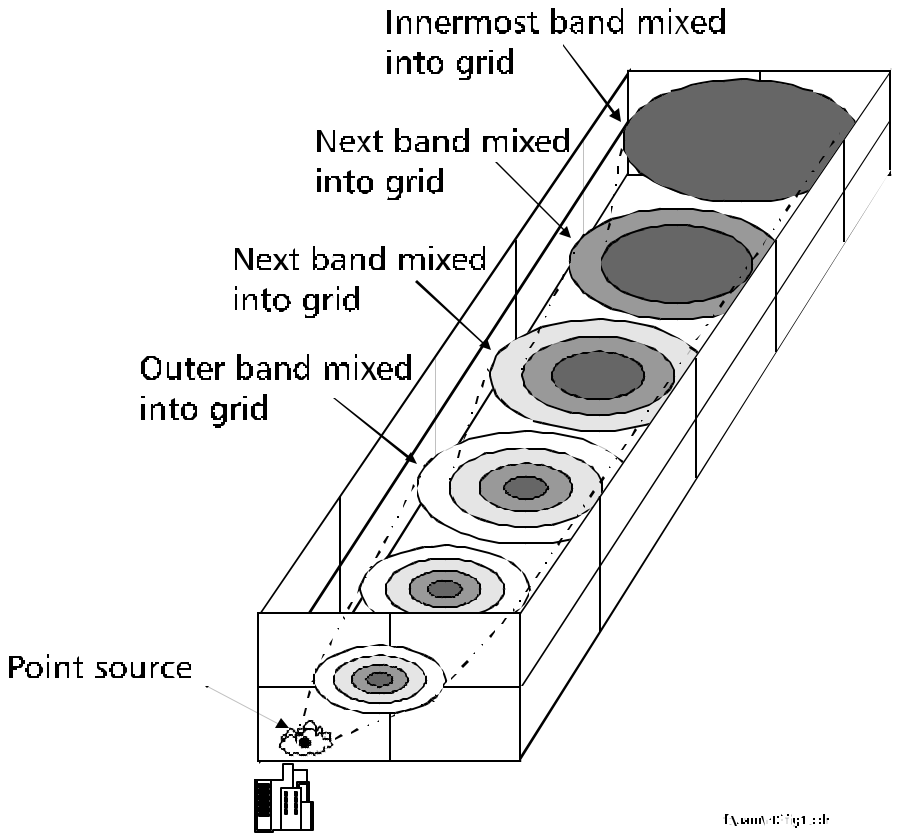
If a puff enters a fine-grid subdomain from a coarser grid, puff mass is shed from a sufficient number of reactor cells to reduce puff size below the size of a fine-grid cell. If a puff crosses from a fine grid into a coarser grid, the puff remains intact until it grows to dimensions commensurate with the coarse grid.

At any single time step during a "typical" UAM-V application (treating 10–20 large NO_x sources with the PiG), hundreds of puffs may accumulate, particularly during the night when stability severely limits plume growth. These puffs can remain highly NO_x-concentrated for a substantial distance downstream, with little or no in-puff ozone production. Integration of the full CB-IV chemical mechanism in this numerically "stiff" situation is time-consuming and unnecessary. Thus a simple equilibrium calculation is provided as an optional replacement of the full CB-IV chemistry. This option may be used for any subset of PiG-treated sources. The method utilizes a modification of the highly condensed and parameterized RIVAD chemical mechanism (Morris et al., 1988). The following are main features of the mechanism:

1. Steady-state (photostationary) chemistry of NO_x and O_3 is assumed during the daytime; titration of NO and O_3 is assumed at night. Thus all NO in a puff is converted to NO_2 once night falls regardless of concentrations of O_3 and NO_3.
2. Daytime gas-phase formation of H_2SO_4 and HNO_3 through reactions of SO_2 and NO_2 with the OH radical is included. OH is assumed to be in a steady state with the reaction of H_2O and excited singlet oxygen atoms from photolysis of O_3. Concentrations of VOC are assumed low.
3. At night NO3 and N2O5 are assumed to be in a steady state with NO2 and O3. The amount of HNO3 formed due to reaction of N2O5 with H2O is deducted from [NO2] directly. Nitrogen is not conserved if NO3 and N2O5 occupy more than a small percentage of total nitrogen. Concentrations of NO3 and N2O5 vary significantly due to variations in concentration levels of oxidants.

4. The amount of HNO3 formed in daytime through reaction of NO2 with OH is deducted from [NOx], and the ratio of NO2 to NO is assumed to be the same as calculated from point (1) above.
5. Given initial concentrations of NO, NO2 and O3, steady-state concentrations of NO, NO2, OH, O3, NO3 and N2O5 are calculated at the beginning of each time step before any nitrogen is deducted, in order to take into account formation of HNO3 (regardless of the length of the time step).

Figure 2-1.
Schematic illustration of the UAM-V plume-in-grid algorithm based on the Reactive Plume Model (RPM)



3. SOFTWARE STRUCTURE

This section presents an overview of the structure of the UAM-V software. Figure 3-1, starting on page 3-23, illustrates the calling structure of the UAM-V model; the highest level routines are on the left while the lowest level routines are on the right. Subroutines appear in the tree in the order in which they appear in the source code. This order may not be identical to the order in which routines are called. In addition, multiple calls to the same routine are not listed.

The following are brief descriptions of the function of each subroutine in the UAM-V version 1.30, dated September, 1999. Certain routines are library routines available on many Unix systems. These routines have the notation "(System)" after their name, and their function is described so that calls to equivalent routines can be substituted.

Routines marked with an asterisk are utilized by the standard chemistry solver. When using UAM-V with super-fast chemistry solver, the routines included are STEP4, PLANB, CHEM, CHEMA, CHEM2A, CHEM2B, and CHEM2AD.

UAMV

Main driving routine for the UAM-V model.

Called by: None

Calls: AVERAG, AVERGF, BDRFIL, CALTOJ, CALVDF, CLVDFF, CRSFIL, CUMPRT, DIFFSF, DTSIZE, EFTOT, EMCORS, EMFINE, FBDFIL, FCMPRT, FGRTRP, FINFIL, FMSCAL, FMSFLO, FMSPRT, FSTEP, FVRTWD, GET_FINAL, GETPT, GETQAR, GUNIT, HEDPTS, HEDQAR, HGTNEW, HTFCAL, INJECT, INJECTF, INTRVL,IRR_INIT0, IRR_INIT1, IRR_WRT, IRR_WRTF, JTOCAL, MASCAL, MASFLO, NDAYAD, NSTFIL, PGWRIT, PLGMAS, PRINTR, PRTINT, RCHEM, RCHEMF, RVMMAP, SETUP, SRLYRF, STEPX, STEPXF, STEPY, STEPYF, SURLYR, TERMSF, TTRAJ, UPDATE, VERTWD, XCMPRT, XMSCAL, XMSFLO, XMSPRT, XTIME, GETARG (System), FLUSH (System)

AERODY

Calculates aerodynamic resistance for dry deposition.

Called by: SRLYRF, SURLYR

Calls: None

AHINTF

Initializes a parameter for aqueous-phase chemistry on fine grids.

Called by: SETUP

Calls: None

ALLOC

Allocates memory from the scratch array for storage of rolling ozone averages.

Called by: SETUP

Calls: None

AMBIEN

Interpolates ambient concentrations at current timestep to PiG chemistry time step.

Called by: EULER

Calls: None

ARRGET

Returns a 1D vector of the column of values located at an *i*,*j* location in a 3D array.

Called by: FBDFIL

Calls: None

AVERAG

Calculates time-averaged concentrations over coarse domain.

Called by: UAMV

Calls: None

AVERGF

Calculates time-averaged concentrations over fine grids.

Called by: UAMV

Calls: None

BD1

Block data, initializes species names and selected data.

Called by: None

Calls: None

BDRFIL

Fills in boundary conditions for a fine grid contained within the coarse domain.

Called by: UAMV

Calls: None

BEH084

Calculates effective stack height from plume rise calculation.

Called by: UPDATE

Calls: FLUSH (System)

BNDDEF

Reads domain boundary definitions from BOUNDARY file.

Called by: SETUP

Calls: None

BNDRY

Calculates laminar boundary layer resistance for dry deposition.

Called by: SRLYRF, SURLYR

Calls: None

CALTOJ

Converts calendar date to Julian date.

Called by: UAMV, GETBC, GETHAZ, GETIC, GETPT, GETQAR, PGREAD, PRINTR, RESTRT, SETUP, UPDATE

Calls: None

CALVDF

Prepares variables for vertical diffusion calculation on the coarse domain.

Called by: UAMV

Calls: None

CHEM*

Calculates daytime chemical reaction rates.

Called by: STEP4

Calls: COLPIVOT, FASTJAC, FASTRATE, FLUSH (System), RADJRAT

CHEMA

Calculates daytime chemical reaction rates for fast solver.

Called by: STEP4F

Calls: COLPIVOT, FASTJAC_A, FASTRATE_A, FLUSH (System), RADJRAT

CHEMS

Calculates daytime reaction rates for steady-state plume chemistry.

Called by: SSDAY

Calls: CHRT1S, CHRT3S, FLUSH (System)

CHEM2A1*

Calculates nighttime chemical reaction rates when there is an excess of O3.

Called by: STEP4

Calls: COLPIVOT, FLUSH (System), FASTJAC_2A1, FASTRATE_2A1, RADJRAT_2A1

CHEM2A1F

Calculates nighttime chemical reaction rates for fast solver when there is an excess of O3.

Called by: STEP4F

Calls: COLPIVOT, FLUSH (System), FASTJAC_2A1F, FASTRATE_2A1F, RADJRAT_2A1F

CHEM2A2*

Calculates nighttime chemical reaction rates for standard solver when there is an excess of NO.

Called by: STEP4

Calls: COLPIVOT, FLUSH (System), FASTJAC_2A2, FASTRATE_2A2, RADJRAT_2A2

CHEM2A2F

Calculates nighttime chemical reaction rates for fast solver when there is an excess of NO.

Called by: STEP4F

Calls: COLPIVOT, FLUSH (System), FASTJAC_2A2F, FASTRATE_2A2F, RADJRAT_2A2F

CHEM2B*

Calculates nighttime chemical reaction rates when NO and O3 are both small.

Called by: STEP4

Calls: COLPIVOT, FASTJAC_2B, FASTRATE_2B, FLUSH (System), RADJRAT_2B

CHEM2BF

Calculates nighttime chemical reaction rates for fast solver when NO and O3 are both small.

Called by: STEP4F

Calls: COLPIVOT, FASTJAC_2BF, FASTRATE_2BF, FLUSH (System), RADJRAT_2BF

CHKDAT

Checks calendar and Julian dates for proper format.

Called by: DIAGN

Calls: None

CHM22S

Alternate calculation for nighttime reaction rates for steady-state plume chemistry. Currently not used.

Called by: None

Calls: None

CHM23S

Calculates nighttime reaction rates for steady-state plume chemistry.

Called by: SSDARK

Calls: None

CHREAD

Reads chemistry parameters and fills species indices.

Called by: SETUP

Calls: FLUSH (System)

CHRT1S

Calculates species rate of change for daytime steady-state plume chemistry with NO3 and N2O5 treated explicitly.

Called by: CHEMS

Calls: None

CHRT3S

Calculates species rate of change for daytime steady-state plume chemistry with NO3 and N2O5 treated via NXOY.

Called by: CHEMS

Calls: None

CKHGT

Checks that the fine grid's layer heights correspond to the coarse grid's layer heights.

Called by: UPDATE

Calls: None

CLLDIM

Calculates PiG onionskin cell width factors.

Called by: PIGINIT

Calls: FINTEG

CLVDFF

Prepares variables for vertical diffusion calculation on a fine grid.

Called by: UAMV

Calls: None

CNVTBC

Convert boundary concentrations in ppm to micromoles/m^3

Called by: UPDATE

Calls: None

COLPIVOT

Solve set of linear equations by Gaussian maximum column's pivot method.

Called by: CHEM, CHEM2A1, CHEM2A2, CHEM2B, CHEM2A1F, CHEM2A2F, CHEM2BF, CHEMA, STEP4, STEP4F

Calls: None

CONVRT

Converts position to grid coordinates.

Called by: EMCORS, EMFINE, PLGMAS, UPDATE

Calls: None

CRSFIL

Fills in coarse-domain concentrations with fine-grid concentrations.

Called by: UAMV

Calls: GET_DIFC

CUMPRT

Prints coarse-domain cumulative mass fluxes at the end of a run.

Called by: UAMV

Calls: None

DELTAZ

Calculates fine-grid cell depth that a PiG puff will occupy next time step.

Called by: PUFFDMP

Calls: None

DEVCON

Calculates cross plume average from PiG cell averages, and vice versa.

Called by: EULER, DOCHEM, INITLZ

Calls: None

DIAGN

Checks input and model-derived parameters against allowable values, and calculates mins, maxs, and averages.

Called by: SETUP, UPDATE

Calls: CHKDAT, FLUSH (System)

DIFFSF

Calculates horizontal diffusion coefficient for fine grids, based on scale considerations and deformation of the windfield.

Called by: UAMV

Calls: None

DIFFUS

Calculates horizontal diffusion coefficient for the coarse domain, based on scale considerations and deformation of the windfield.

Called by: UPDATE

Calls: None

DMPPIG

Dumps the mass for a single puff in preparation for save to external file.

Called by: PIGDMP

Calls: None

DOCHEM

Driver for PiG chemistry routines.

Called by: RPM

Calls: PHOT, TDRATE, STEP4, STEP4F, DEVCON, SSDARK, SSDAY

DTSIZE

Determines time step for the coarse domain.

Called by: UAMV

Calls: None

EFTOT

Sums area sources over a fine grid and write totals.

Called by: UAMV, SETUP

Calls: None

EMCORS

Injects point and area source emissions into the coarse domain.

Called by: UAMV

Calls: CONVRT, GET_DIFC

EMFINE

Injects point and area source emissions into the fine grids.

Called by: UAMV

Calls: CONVRT

ENDIND

Determines ending indices for aggregate cell.

Called by: RVMMAP

Calls: None

EULER

Advances PiG plume cross-sections one time step downwind.

Called by: RPM

Calls: AMBIEN, DEVCON

EXPAND

Expands PiG puff based on Pasquill-Gifford stability class over the depth of the puff in the coarse domain. Also controls vertical growth of plume, and limits puff volume to a fraction of grid-cell volume.

Called by: TTRAJ

Calls: SIGMAY, SIGMAZ

EXPANDF

Expands PiG puff based on Pasquill-Gifford stability class over the depth of the puff in a fine grid. Also controls vertical growth of plume, and limits puff volume to a fraction of grid-cell volume.

Called by: TTRAJ

Calls: SIGMAY, SIGMAZ

FASTJAC

Calculate jacobian elements for fast reacting species.

Called by: CHEM

Calls: None

FASTJAC_A

Calculate jacobian elements for fast reacting species in fast solver.

Called by: CHEMA

Calls: None

FASTJAC_2A1

Calculate jacobian elements for fast reacting species during nighttime excess O3 conditions.

Called by: CHEM2A1

Calls: None

FASTJAC_2A1F

Calculate jacobian elements for fast reacting species during nighttime excess O3 conditions for fast solver.

Called by: CHEM2A1F

Calls: None

FASTJAC_2A2

Calculate jacobian elements for fast reacting species during nighttime excess NO conditions.

Called by: CHEM2A2

Calls: None

FASTJAC_2A2F

Calculate jacobian elements for fast reacting species during nighttime excess NO conditions for fast solver.

Called by: CHEM2A2F

Calls: None

FASTJAC_2B

Calculate jacobian elements for fast reacting species during nighttime when NO and O3 are both small.

Called by: CHEM2B

Calls: None

FASTJAC_2BF

Calculate jacobian elements for fast reacting species during nighttime when NO and O3 are both small for fast solver.

Called by: CHEM2BF

Calls: None

FASTRATE

Calculate rates for fast reacting species.

Called by: CHEM

Calls: None

FASTRATE_2A1

Calculate rates for fast reacting species during nighttime when there is an excess of O3.

Called by: CHEM2A1

Calls: None

FASTRATE_2A1F

Calculate rates for fast reacting species during nighttime when there is an excess of O3 for fast solver.

Called by: CHEM2A1F

Calls: None

FASTRATE_2A2

Calculate rates for fast reacting species during nighttime when there is an excess of NO.

Called by: CHEM2A2

Calls: None

FASTRATE_2A2F

Calculate rates for fast reacting species during nighttime when there is an excess of NO for fast solver.

Called by: CHEM2A2F

Calls: None

FASTRATE_2B

Calculate rates for fast reacting species during nighttime when NO and O3 are both small.

Called by: CHEM2B

Calls: None

FASTRATE_2BF

Calculate rates for fast reacting species during nighttime when NO and O3 are both small for fast solver.

Called by: CHEM2BF

Calls: None

FASTRATE_A

Calculate rates for fast reacting species for fast solver.

Called by: CHEMA

Calls: None

FBDFIL

Fills in boundary conditions for a fine grid contained within another fine grid.

Called by: UAMV

Calls: ARRGET

FCMPRT

Prints fine-grid cumulative mass flux across region boundaries at end of run.

Called by: UAMV

Calls: None

FFGTRP

Interpolates data onto a fine grid from data for another fine grid.

Called by: UPDATE

Calls: REDUCR

FGAVWR

Writes time-averaged fine-grid concentrations to a binary file.

Called by: PRINTR

Calls: None

FGMAX

Calculates maximum u and v wind components on a fine grid.

Called by: FSTEP

Calls: None

FGREAD

Reads instantaneous fine-grid concentrations from a binary file.

Called by: RESTRT

Calls: None

FGRTRP

Interpolates coarse domain data to a fine grid.

Called by: UAMV, UPDATE

Calls: None

FGWRIT

Writes instantaneous fine-grid concentrations to a binary file.

Called by: PRINTR, PRTINT

Calls: None

FINFIL

Fills in a fine grid with coarse-domain concentrations for initial conditions.

Called by: UAMV

Calls: None

FINTEG

Calculates fraction of mass in a two-dimensional Gaussian hill.

Called by: CLLDIM

Calls: None

FKINDX

Determine a fine grid z-index corresponding to a height.

Called by: TTRAJ

Calls: None

FLUSH (System)

Called with an argument of n forces any memory buffers for Fortran unit n to be written to disk. If an equivalent routine is unavailable, calls to this routine may be removed.

Called by: UAMV, BEH084, CHEM2A1, CHEM2A2, CHEM2B, CHEM, CHEM2A1F, CHEM2A2F, CHEM2BF, CHEMA, CHREAD, DIAGN, IRR_CONC, IRR_WRT, IRR_WRTF, PGWRIT, PRINTR, PRTINT, PIGDMP, CHEMS, STEP4, STEP4F

FLXNIT

Initializes all mass flux tracking arrays to zero.

Called by: SETUP

Calls: None

FMSCAL

Calculates mass budget for a fine grid.

Called by: UAMV

Calls: None

FMSFLO

Calculates mass flux across fine-grid region boundaries.

Called by: UAMV

Calls: None

FMSPRT

Prints mass flux across fine-grid region boundaries.

Called by: UAMV

Calls: None

FSTEP

Determines maximum time step for a fine grid, and the number of time steps to complete one coarse-domain time step.

Called by: UAMV

Calls: FGMAX

FVRTWD

Calculates effective vertical wind on a fine grid due to divergence and changing layer depths.

Called by: UAMV

Calls: None

GETARG (System)

Called with a first argument of n, returns as its second argument (a character variable) the string that is the nth parameter on the UAM-V command line. This routine is used by UAM-V to set the name of the control file (FN) and to set the value of IDEBUG, the diagnostic flag. If an equivalent routine is not available on the system being used, the code must be rewritten to set FN and IDEBUG in some other way.

Called by: UAMV

GETBC

Reads coarse-domain boundary conditions for a particular time interval.

Called by: UPDATE

Calls: CALTOJ, INTRVL

GET_DIFC

Calculate the change in concentration due to an individual process.

Called by: CRSFIL, EMCORS, INJECT, RCHEM

Calls: IRR_CONC

GET_FINAL

Save final concentration at end of step for process analysis.

Called by: UAMV

Calls: None

GETHAZ

Reads one data interval from albedo/haze/ozone column file.

Called by: UPDATE

Calls: CALTOJ, LFTPAK, INTRVL

GETIC

Reads coarse-domain initial conditions.

Called by: SETUP

Calls: CALTOJ, INTRVL

GETPT

Reads point-source emissions information for a particular time interval.

Called by: UAMV, SETUP

Calls: CALTOJ, INTRVL

GETQAR

Reads area-source emissions information for a particular time interval.

Called by: UAMV, SETUP

Calls: CALTOJ, INTRVL

GRDSP

Determines cell sizes, cell center locations for fine grids and coarse domain.

Called by: SETUP

Calls: None

GUNIT

Returns unit number for area emissions file depending on the day of the week.

Called by: UAMV, SETUP

Calls: JTOCAL, ZELLAR

GXYWR

Write a grid of values to a file.

Called by: PRINTR

Calls: None

HDRCHK

Read meteorological file headers and check values against domain values.

Called by: SETUP, UPDATE

Calls: None

HEDDV

Reads header of deposition velocity file.

Called by: SETUP

Calls: None

HEDIBC

Reads header of initial conditions file.

Called by: SETUP

Calls: None

HEDPTS

Reads header of point-source emissions file.

Called by: UAMV, SETUP

Calls: None

HEDQAR

Reads header of area emissions file.

Called by: UAMV, SETUP

Calls: None

HGTNEW

Updates values of coarse-grid layer heights to current time.

Called by: UAMV

Calls: None

HTFAGE

Replaces old fine-grid height array with values in new height array in preparation for reading in new data.

Called by: UPDATE

Calls: None

HTFCAL

Calculates layer interface heights current time step for a fine grid.

Called by: UAMV

Calls: None

INITLZ

Initializes a PiG puff when it is first released, filling it with emissions in a Gaussian distribution.

Called by: RPM

Calls: DEVCON

INJECT

Injects mass from PiG puffs into the coarse domain.

Called by: UAMV

Calls: GET_DIFC

INJECTF

Injects mass from PiG puffs into the fine grids.

Called by: UAMV

Calls: None

INTRVL

Calculate number of days between two dates.

Called by: UAMV, GETBC, GETHAZ, GETIC, GETPT, GETQAR, PGREAD, RESTRT, RVMMAP, UPDATE

Calls: None

IRR_CONC

Sum changes in coarse grid concentrations due to PiG, point sources, area sources, chemistry, or fine grid fill-in.

Called by: GET_DIFC

Calls: FLUSH (System)

IRR_INIT0

Initialize coarse and fine grid process analysis arrays to zero.

Called by: UAMV

Calls: None

IRR_INIT1

Read in definition of process analysis area and initialize process analysis variables.

Called by: UAMV

Calls: None

IRR_RATE

Store final reaction rates for PA/IRR treatment. (Not currently implemented.)

Called by: STEP4

Calls: None

IRR_WRT

Write coarse grid process analysis data.

Called by: UAMV

Calls: FLUSH (System)

IRR_WRTF

Write fine grid process analysis data.

Called by: UAMV

Calls: FLUSH (System)

JTOCAL

Converts Julian date to calendar date.

Called by: UAMV, GUNIT, PRINTR, RCHEM, RCHEMF, RPM, SRLYRF, SURLYR, TERMS, TERMSF, UPDATE

Calls: None

LFTPAK

Packs all text to the left.

Called by: GETHAZ, SETUP, UPDATE

Calls: None

MASCAL

Calculates a mass budget for the coarse domain.

Called by: UAMV

Calls: None

MASFLO

Calculates mass flux across coarse-domain region boundaries.

Called by: UAMV

Calls: None

NDAYAD

Adds 1 to calendar date.

Called by: UAMV

Calls: None

NDAYSUB

Subtract 1 from the calendar date.

Called by: PRINTR

Calls: None

NSTFIL

Fills in a fine grid's concentrations with those from nested fine grids.

Called by: UAMV

Calls: None

PBLMOD

Calculates PBL parameters from similarity theory.

Called by: SURLYR, SRLYRF

Calls: None

PGREAD

Reads instantaneous PiG information for model restart.

Called by: SETUP

Calls: CALTOJ, INTRVL, PIGDMP

PGWRIT

Writes instantaneous PiG information to a file for future restart.

Called by: UAMV

Calls: PIGDMP, FLUSH (System)

PHOT

Determines photolysis rate constant for a particular cell in the coarse domain.

Called by: RCHEM, DOCHEM

Calls: SOLAR

PHOTF

Determines photolysis rate constant for a particular cell in a fine grid.

Called by: RCHEMF

Calls: SOLAR

PIGDMP

Saves data for puffs to external file for use in postprocessing to prepare boundary condition files for sub-domains.

Called by: PGREAD, PGWRIT, SETUP

Calls: DMPPIG, FLUSH (System)

PIGINIT

Initializes PiG parameters.

Called by: SETUP

Calls: CLLDIM

PLGMAS

Calculates total emissions from PiG sources during a coarse-grid time step.

Called by: UAMV

Calls: CONVRT

PRINTR

Writes out instantaneous and time-averaged concentrations for fine grids and coarse domain.

Called by: UAMV

Calls: CALTOJ, FGAVWR, FGWRIT, GXYWR, JTOCAL, NDAYSUB, FLUSH (System)

PRTDEP

Estimates aerosol dry deposition velocities from a defined mass distribution.

Called by: SURLYR, SRLYRF

Calls: SEDRAT, STOKE, SHMIDT

PRTINT

Writes initial concentrations to INSTANT file.

Called by: UAMV

Calls: FGWRIT, FLUSH (System)

PUFFDMP

Determines whether a PiG puff should dump some or all of its mass into the fine and/or coarse grids, and calculates mass, volume, time, and grid cells for dumping.

Called by: TTRAJ

Calls: DELTAZ

RADJRAT

Calculate Jacobian for radical species.

Called by: CHEM, CHEMA

Calls: None

RADJRAT_2A1

Calculate Jacobian for radical species in nighttime standard solver chemistry

Called by: CHEM2A1

Calls: None

RADJRAT_2A1F

Calculate Jacobian for radical species in nighttime fast solver chemistry.

Called by: CHEM2A1F

Calls: None

RADJRAT_2A2

Calculate Jacobian for radical species in nighttime standard solver when there is an excess of NO.

Called by: CHEM2A2

Calls: None

RADJRAT_2A2F

Calculate Jacobian for radical species in nighttime fast solver when there is an excess of NO.

Called by: CHEM2A2F

Calls: None

RADJRAT_2B

Calculate Jacobian for radical species in nighttime standard solver when NO and O3 are both small.

Called by: CHEM2B

Calls: None

RADJRAT_2BF

Calculate Jacobian for radical species in nighttime fast solver when NO and O3 are both small.

Called by: CHEM2BF

Calls: None

RCHEM

Chemistry driver for the coarse domain.

Called by: UAMV

Calls: GET_DIFC, JTOCAL, PHOT, STEP4, STEP4F, TDRATE

RCHEMF

Chemistry driver for the fine grids.

Called by: UAMV

Calls: JTOCAL, PHOTF, STEP4, STEP4F, TDRATE

RDFCLD

Reads fine-grid cloud data records.

Called by: UPDATE

Calls: None

RDFH2O

Reads fine-grid water vapor data records.

Called by: UPDATE

Calls: None

RDFKV

Reads fine-grid vertical diffusivity fields for a particular time interval.

Called by: UPDATE

Calls: None

RDFRN

Reads fine-grid rain data records.

Called by: UPDATE

Calls: None

RDFSRF

Reads fine-grid surface data.

Called by: SETUP

Calls: None

RDFTMP

Reads fine-grid temperature data records.

Called by: UPDATE

Calls: None

RDFWND

Reads fine-grid wind fields for a particular time interval.

Called by: UPDATE

Calls: None

RDFZP

Reads one time interval of fine-grid height file and converts to internal units.

Called by: UPDATE

Calls: None

REDUCR

Removes common factors from two integer values.

Called by: FFGTRP

Calls: None

RESTRT

Reads instantaneous concentration files to initialize fine- and coarse-grid concentration fields.

Called by: SETUP

Calls: CALTOJ, FGREAD, INTRVL

RPM

Driver for the Reactive Plume Model (RPM) routines within the PiG model.

Called by: TTRAJ

Calls: EULER, DOCHEM, SWITCH, INITLZ, JTOCAL

RVMMAP

Reads in aggregation/nesting maps to determine positions, sizes, and orientations of aggregated cells and nested grids within the coarse domain.

Called by: SETUP, UAMV

Calls: ENDIND, INTRVL

SEDRAT

Estimates particulate sedimentation velocity.

Called by: PRTDEP

Calls: None

SETPRM

Sets PiG puff-dependent variables for RPM.

Called by: TTRAJ

Calls: None

SETUP

Controls initialization of model run: opens data files, reads file headers if applicable, synchronizes data files, positions data files to beginning of run, reads initial time interval of data.

Called by: UAMV

Calls: AHINTF, ALLOC, BNDDEF, CALTOJ, CHREAD, DIAGN, EFTOT, FLXNIT, GETIC, GETPT, GETQAR, GRDSP, GUNIT, HDRCHK, HEDDV, HEDIBC, HEDPTS, HEDQAR, LFTPAK, PGREAD, PIGINIT, PIGDMP, RDFSRF, RESTRT, RVMMAP, TIRATE, UNCHEK, UPDATE

SHMIDT

Calculates the Schmidt number for dry particulate deposition.

Called by: PRTDEP

Calls: None

SIGMAY

Determines horizontal standard deviation of a Gaussian-shaped plume to define PiG puff size.

Called by: EXPAND, EXPANDF

Calls: None

SIGMAZ

Determines vertical standard deviation of a Gaussian-shaped plume to define PiG puff size.

Called by: EXPAND, EXPANDF

Calls: None

SLOWDR

Calculate rates and jacobian elements for slow reacting species for fast solver.

Called by: STEP4F

Calls: None

SLOWNTA1

Calculate rates and jacobian elements for fast solver during nighttime when O3 is small.

Called by: STEP4F

Calls: None

SLOWNTA2

Calculate rates and jacobian elements for fast solver during nighttime when NO is small.

Called by: STEP4F

Calls: None

SLOWNTB

Calculate rates and jacobian elements for fast solver during nighttime when O3 and NO are small.

Called by: STEP4F

Calls: None

SMOLAR

Performs horizontal advection using the Smolarkiewicz scheme.

Called by: STEPX, STEPXF, STEPY, STEPYF

Calls: None

SOLAR

Calculates solar zenith angle based on date, time, and lat/lon.

Called by: TERMS, PHOT, PHOTF, SURLYR, SRLYRF, TERMSF

Calls: None

SRLYRF

Calculates dry deposition velocities for fine grids.

Called by: UAMV

Calls: SOLAR, PBLMOD, AERODY, BNDRY, PRTDEP, SURFCE, JTOCAL

SSDARK

Nighttime steady-state plume chemistry.

Called by: DOCHEM

Calls: CHM23S

SSDAY

Daytime steady-state plume chemistry.

Called by: DOCHEM

Calls: CHEMS

STEP4*

Performs chemistry for one time step in one cell.

Called by: DOCHEM, RCHEM, RCHEMF

Calls: CHEM, CHEM2A1, CHEM2A2, CHEM2B, IRR_RATE, COLPIVOT, TITRAT, FLUSH (System)

STEP4F

Performs chemistry for one time step in one cell using fast solver.

Called by: DOCHEM, RCHEM, RCHEMF

Calls: CHEMA, CHEM2A1F, CHEM2A2F, CHEM2BF, COLPIVOT, SLOWDR, SLOWNTA1, SLOWNTA2, SLOWNTB, TITRAT, FLUSH (System)

STEPX

Prepares variables for x-advection calculation on coarse domain.

Called by: UAMV

Calls: SMOLAR, TERMS

STEPXF

Prepares variables for x-advection calculation on a fine grid.

Called by: UAMV

Calls: SMOLAR

STEPY

Prepares variables for y-advection calculation on coarse domain.

Called by: UAMV

Calls: SMOLAR

STEPYF

Prepares variables for y-advection calculation on a fine grid.

Called by: UAMV

Calls: SMOLAR

STOKE

Calculates the Stoke number for dry particulate deposition.

Called by: PRTDEP

Calls: None

SURFCE

Calculates surface layer resistance for dry deposition.

Called by: SURLYR, SRLYRF

Calls: TDRATE, VAPSRC

SURLYR

Gaseous/particulate dry deposition driver, calculates gaseous dry deposition velocities.

Called by: UAMV

Calls: SOLAR, PBLMOD, AERODY, BNDRY, PRTDEP, SURFCE, JTOCAL

SWITCH

Dumps current PiG puff information into 'old' arrays.

Called by: RPM

Calls: None

TDRATE

Adjusts chemical rate constants for temperature and pressure.

Called by: DOCHEM, RCHEM, RCHEMF, SURFCE

Calls: None

TERMS

Calculates wet deposition and linear SO2/SO4 chemical reaction rates on the coarse domain.

Called by: STEPX

Calls: SOLAR, WETDEP, JTOCAL

TERMSF

Calculates wet deposition and linear SO_2/SO_4 chemical reaction rates on the fine grids.

Called by: UAMV

Calls: SOLAR, WETDEPF, JTOCAL

TIRATE

Fills look-up table for temperature-dependent rate constants.

Called by: SETUP

Calls: None

TITRAT

Calculates steady-state concentrations of NO_x and O_3 at night by mathematical titration.

Called by: STEP4, STEP4F

Calls: None

TRJSTP

Determines for each PiG puff the time step, distance traveled over that time step, and new 3-dimensional position in terms of km and grid indices on fine or coarse domains.

Called by: TTRAJ

Calls: None

TTRAJ

Driver for the plume-in-grid (PiG) / reactive plume model (RPM) treatment.

Called by: UAMV

Calls: TRJSTP, SETPRM, PUFFDMP, RPM, EXPAND, EXPANDF, FKINDX

UNCHEK

Checks for multiple use of same output unit number.

Called by: SETUP

Calls: None

UPDATE

Controls the updating/reading of environmental inputs over specific time intervals.

Called by: SETUP, UAMV

Calls: BEH084, CONVRT, CALTOJ, CKHGT, CNVTBC, DIFFUS, DIAGN, FFGTRP, FGRTRP, GETBC, GETHAZ, HDRCHK, HTFAGE, INTRVL, JTOCAL, LFTPAK, RDFCLD, RDFH2O, RDFTMP, RDFKV, RDFRN, RDFWND, RDFZP

VAPSRC

Calculates the equilibrium vapor pressure of water.

Called by: SURFCE

Calls: None

VERTWD

Calculates effective coarse-grid vertical wind due to wind field divergence and temporal change of layer heights.

Called by: UAMV

Calls: None

WETDEP

Calculates a decay rate for all species due to precipitation scavenging on the coarse domain.

Called by: TERMS

Calls: None

WETDEPF

Calculates a decay rate for all species due to precipitation scavenging on a fine grid.

Called by: TERMSF

Calls: None

XCMPRT

At end of run, prints cumulative mass flux across fine-grid region boundaries based on coarse-grid variables.

Called by: UAMV

Calls: None

XMSCAL

Calculates total species mass within fine-grid areas based on coarse-grid variables.

Called by: UAMV

Calls: None

XMSFLO

Calculates mass flux across fine-grid region boundaries based on coarse-grid variables.

Called by: UAMV

Calls: None

XMSPRT

Prints mass flux across fine-grid region boundaries based on coarse-grid variables.

Called by: UAMV

Calls: None

XTIME

Performs arithmetic operations involving time in minutes, and times based on 2400-hour clock.

Called by: UAMV

Calls: None

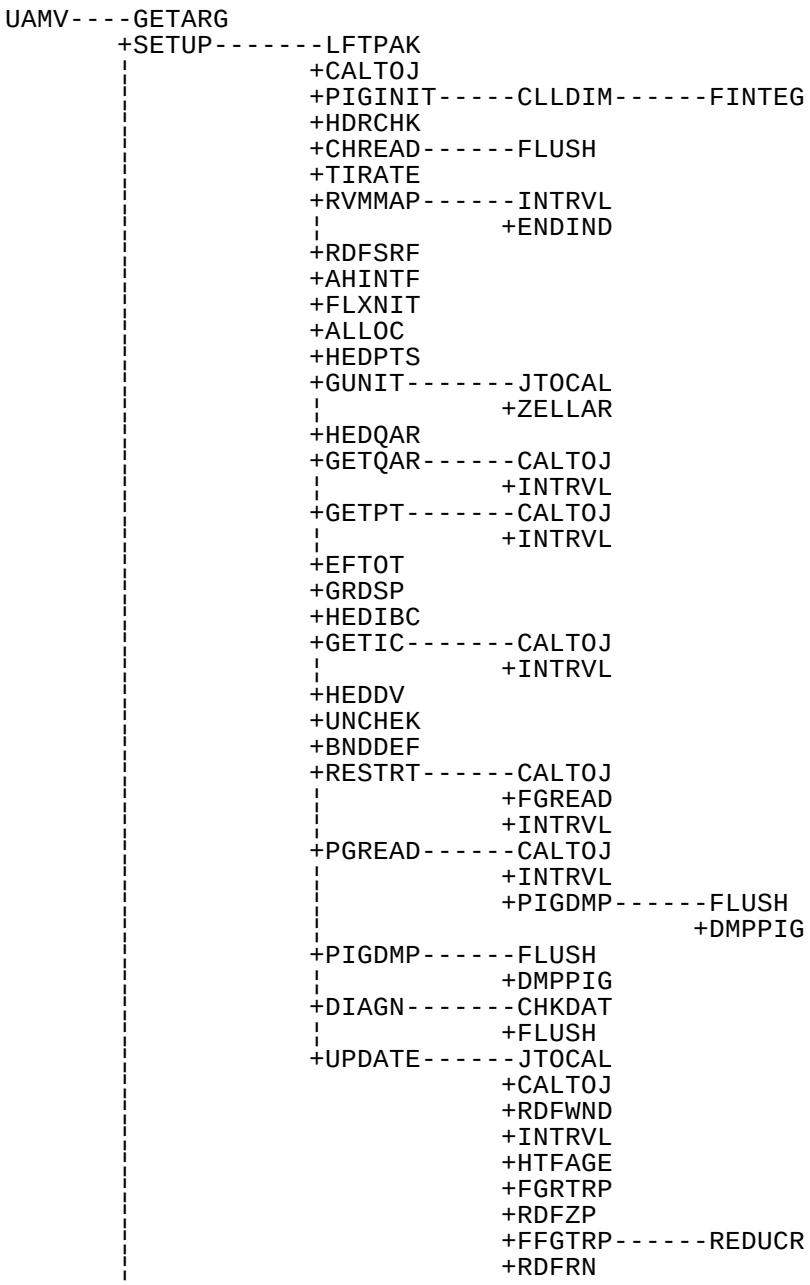
ZELLAR

Determines day of the week given calendar date.

Called by: GUNIT

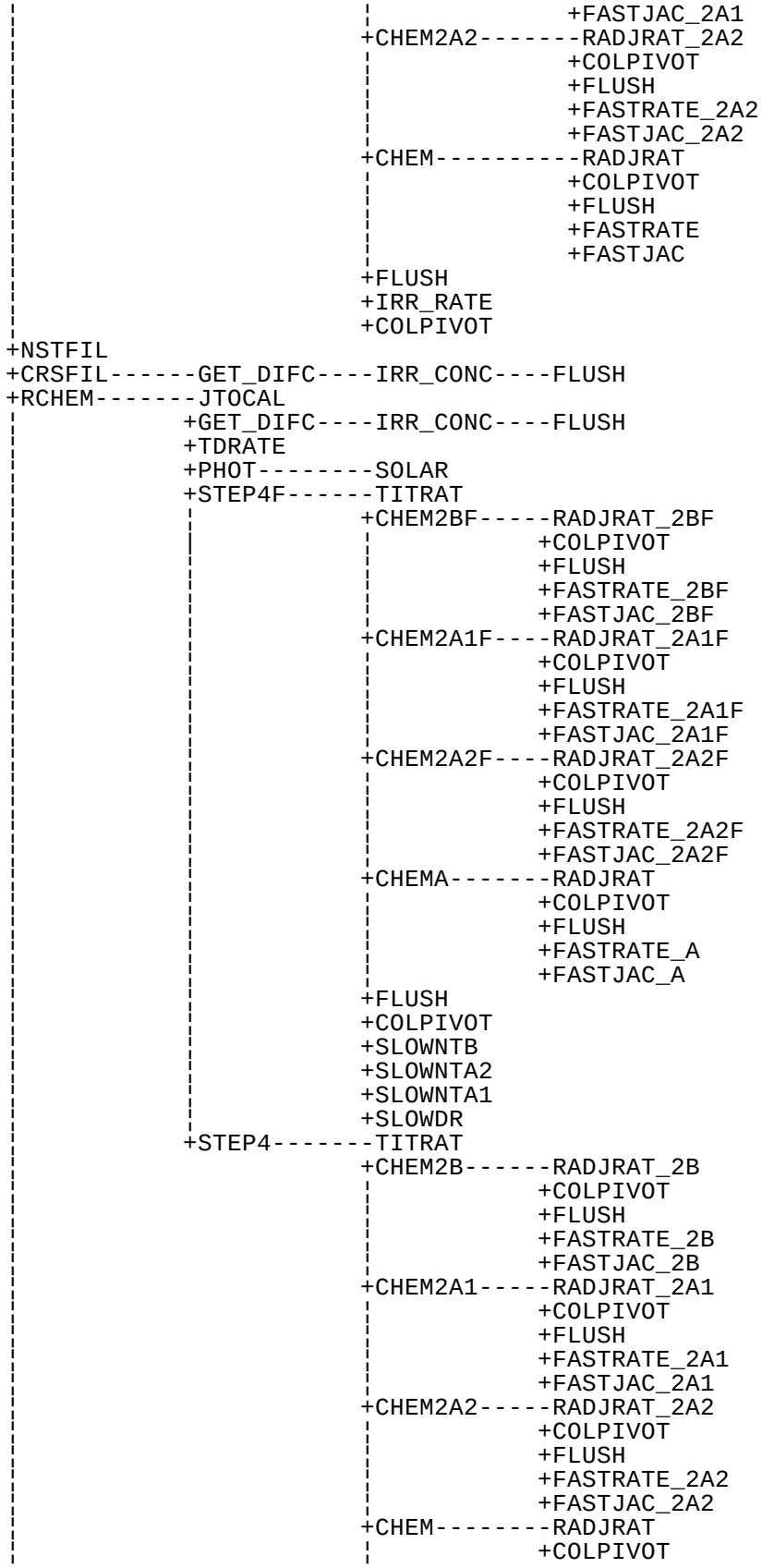
Calls: None

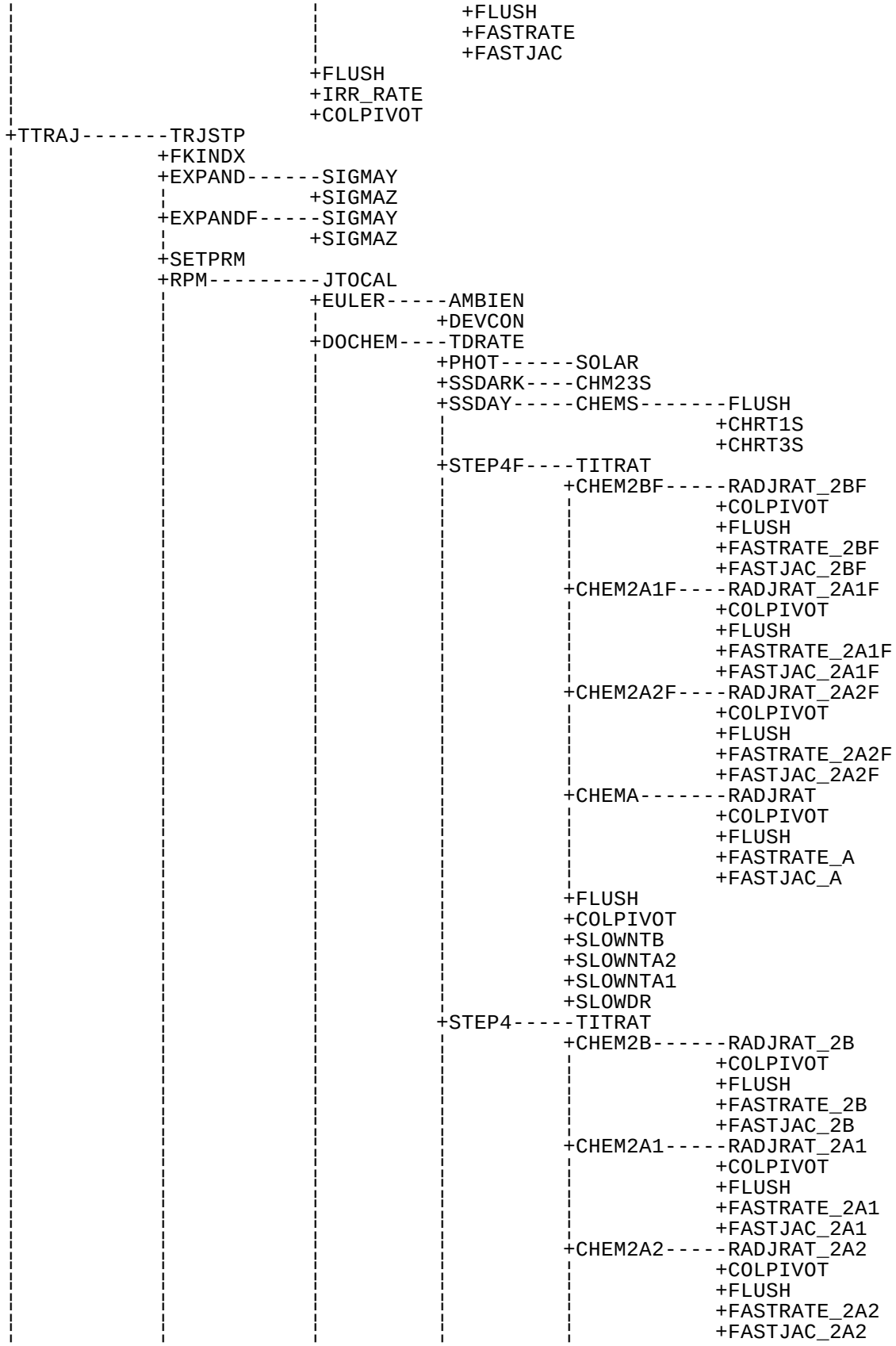
Figure 3-1.
Calling tree for UAM-V, version 1.30, October 25, 1999

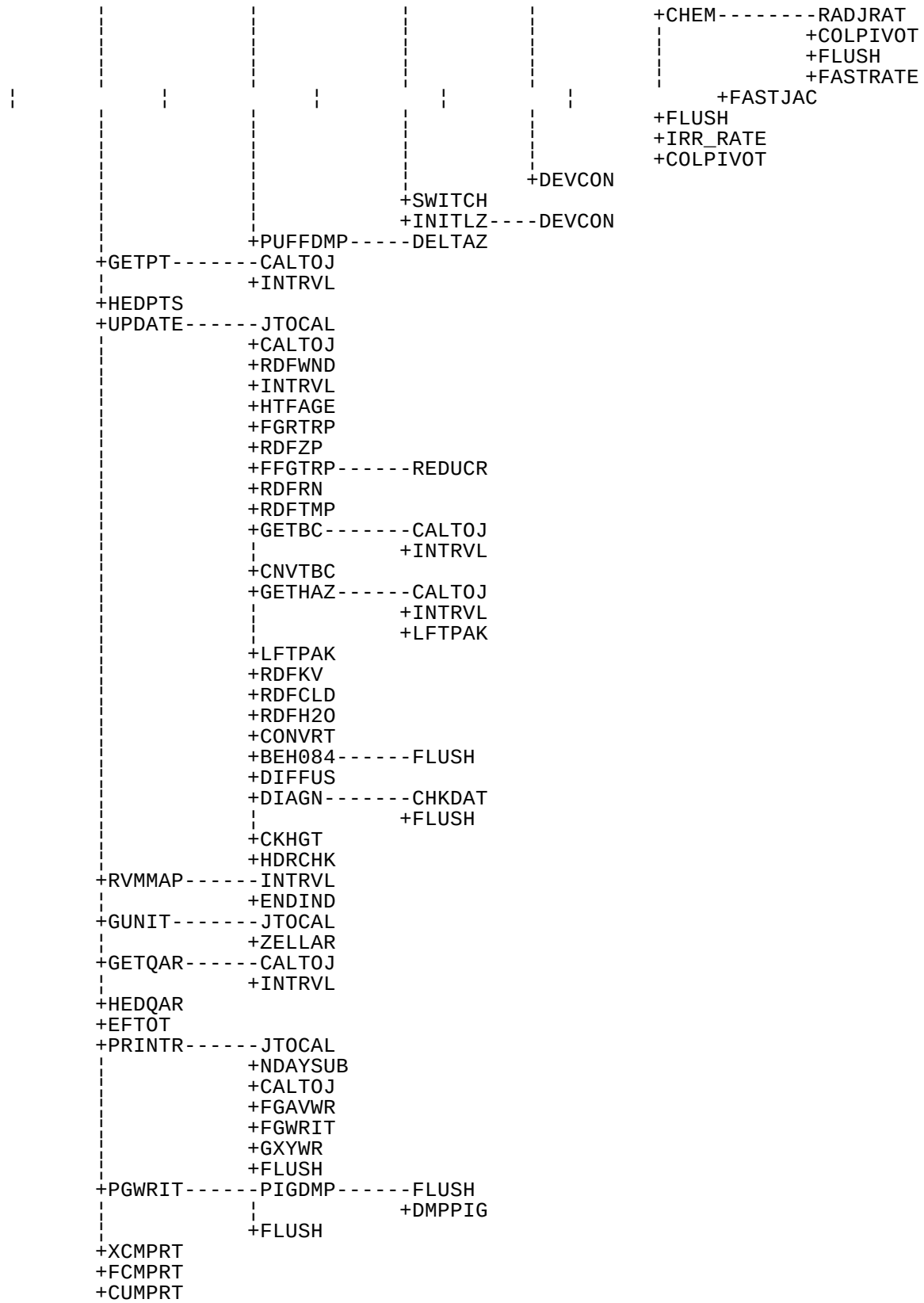


```
|                        +RDFTMP
|                        +GETBC-------CALTOJ
|                        |           +INTRVL
|                        +CNVTBC
|                        +GETHAZ------CALTOJ
|                        |           +INTRVL
|                        |           +LFTPAK
|                        +LFTPAK
|                        +RDFKV
|                        +RDFCLD
|                        +RDFH2O
|                        +CONVRT
|                        +BEH084------FLUSH
|                        +DIFFUS
|                        +DIAGN-------CHKDAT
|                        |           +FLUSH
|                        +CKHGT
|                        +HDRCHK
+FLUSH
+IRR_INIT0
+IRR_INIT1
+FINFIL
+FGRTRP
+PRTINT------FGWRIT
|            +FLUSH
+SURLYR------JTOCAL
|            +SOLAR
|            +PBLMOD
|            +AERODY
|            +BNDRY
|            +PRTDEP------SEDRAT
|            |            +STOKE
|            |            +SHMIDT
|            +SURFCE------TDRATE
|                         +VAPSRC
+SRLYRF------JTOCAL
|            +SOLAR
|            +PBLMOD
|            +AERODY
|            +BNDRY
|            +PRTDEP------SEDRAT
|            |            +STOKE
|            |            +SHMIDT
|            +SURFCE------TDRATE
|                         +VAPSRC
+DTSIZE
+AVERAG
+AVERGF
+GET_FINAL
+IRR_WRT-----FLUSH
+IRR_WRTF----FLUSH
+XTIME
+JTOCAL
+NDAYAD
+CALTOJ
+INTRVL
+MASCAL
+FMSCAL
+XMSCAL
+XMSPRT
+FMSPRT
+MASFLO
+PLGMAS------CONVRT
+INJECT------GET_DIFC----IRR_CONC----FLUSH
+EMCORS------GET_DIFC----IRR_CONC----FLUSH
```

```
|           +CONVRT
+HGTNEW
+VERTWD
+BDRFIL
+XMSFLO
+STEPX-------TERMS-------JTOCAL
|            |           +SOLAR
|            |           +WETDEP
|            +SMOLAR
+STEPY-------SMOLAR
+CALVDF
+FSTEP-------FGMAX
+DIFFSF
+HTFCAL
+FVRTWD
+INJECTF
+EMFINE------CONVRT
+FMSFLO
+FBDFIL------ARRGET
+TERMSF------JTOCAL
|            +SOLAR
|            +WETDEPF
+STEPXF------SMOLAR
+STEPYF------SMOLAR
+CLVDFF
+RCHEMF------JTOCAL
|            +TDRATE
|            +PHOTF-------SOLAR
|            +STEP4F------TITRAT
|            |             +CHEM2BF-----RADJRAT_2BF
|            |             |            +COLPIVOT
|            |             |            +FLUSH
|            |             |            +FASTRATE_2BF
|            |             |            +FASTJAC_2BF
|            |             +CHEM2A1F----RADJRAT_2A1F
|            |             |            +COLPIVOT
|            |             |            +FLUSH
|            |             |            +FASTRATE_2A1F
|            |             |            +FASTJAC_2A1F
|            |             +CHEM2A2F----RADJRAT_2A2F
|            |             |            +COLPIVOT
|            |             |            +FLUSH
|            |             |            +FASTRATE_2A2F
|            |             |            +FASTJAC_2A2F
|            |             +CHEMA-------RADJRAT
|            |             |            +COLPIVOT
|            |             |            +FLUSH
|            |             |            +FASTRATE_A
|            |             |            +FASTJAC_A
|            |             +FLUSH
|            |             +COLPIVOT
|            |             +SLOWNTB
|            |             +SLOWNTA2
|            |             +SLOWNTA1
|            |             +SLOWDR
|            +STEP4-------TITRAT
|                          +CHEM2B--------RADJRAT_2B
|                          |              +COLPIVOT
|                          |              +FLUSH
|                          |              +FASTRATE_2B
|                          |              +FASTJAC_2B
|                          +CHEM2A1-------RADJRAT_2A1
|                          |              +COLPIVOT
|                          |              +FLUSH
|                          |              +FASTRATE_2A1
```


+FASTJAC_2A1
+CHEM2A2-------RADJRAT_2A2
+COLPIVOT
+FLUSH
+FASTRATE_2A2
+FASTJAC_2A2
+CHEM----------RADJRAT
+COLPIVOT
+FLUSH
+FASTRATE
+FASTJAC
+FLUSH
+IRR_RATE
+COLPIVOT
+NSTFIL
+CRSFIL------GET_DIFC----IRR_CONC----FLUSH
+RCHEM-------JTOCAL
+GET_DIFC----IRR_CONC----FLUSH
+TDRATE
+PHOT--------SOLAR
+STEP4F------TITRAT
+CHEM2BF-----RADJRAT_2BF
+COLPIVOT
+FLUSH
+FASTRATE_2BF
+FASTJAC_2BF
+CHEM2A1F----RADJRAT_2A1F
+COLPIVOT
+FLUSH
+FASTRATE_2A1F
+FASTJAC_2A1F
+CHEM2A2F----RADJRAT_2A2F
+COLPIVOT
+FLUSH
+FASTRATE_2A2F
+FASTJAC_2A2F
+CHEMA-------RADJRAT
+COLPIVOT
+FLUSH
+FASTRATE_A
+FASTJAC_A
+FLUSH
+COLPIVOT
+SLOWNTB
+SLOWNTA2
+SLOWNTA1
+SLOWDR
+STEP4-------TITRAT
+CHEM2B------RADJRAT_2B
+COLPIVOT
+FLUSH
+FASTRATE_2B
+FASTJAC_2B
+CHEM2A1-----RADJRAT_2A1
+COLPIVOT
+FLUSH
+FASTRATE_2A1
+FASTJAC_2A1
+CHEM2A2-----RADJRAT_2A2
+COLPIVOT
+FLUSH
+FASTRATE_2A2
+FASTJAC_2A2
+CHEM--------RADJRAT
+COLPIVOT


+FLUSH
+FASTRATE
+FASTJAC
+FLUSH
+IRR_RATE
+COLPIVOT
+TTRAJ-------TRJSTP
+FKINDX
+EXPAND------SIGMAY
+SIGMAZ
+EXPANDF-----SIGMAY
+SIGMAZ
+SETPRM
+RPM---------JTOCAL
+EULER-----AMBIEN
+DEVCON
+DOCHEM----TDRATE
+PHOT------SOLAR
+SSDARK----CHM23S
+SSDAY-----CHEMS-------FLUSH
+CHRT1S
+CHRT3S
+STEP4F----TITRAT
+CHEM2BF-----RADJRAT_2BF
+COLPIVOT
+FLUSH
+FASTRATE_2BF
+FASTJAC_2BF
+CHEM2A1F----RADJRAT_2A1F
+COLPIVOT
+FLUSH
+FASTRATE_2A1F
+FASTJAC_2A1F
+CHEM2A2F----RADJRAT_2A2F
+COLPIVOT
+FLUSH
+FASTRATE_2A2F
+FASTJAC_2A2F
+CHEMA-------RADJRAT
+COLPIVOT
+FLUSH
+FASTRATE_A
+FASTJAC_A
+FLUSH
+COLPIVOT
+SLOWNTB
+SLOWNTA2
+SLOWNTA1
+SLOWDR
+STEP4-----TITRAT
+CHEM2B------RADJRAT_2B
+COLPIVOT
+FLUSH
+FASTRATE_2B
+FASTJAC_2B
+CHEM2A1-----RADJRAT_2A1
+COLPIVOT
+FLUSH
+FASTRATE_2A1
+FASTJAC_2A1
+CHEM2A2-----RADJRAT_2A2
+COLPIVOT
+FLUSH
+FASTRATE_2A2
+FASTJAC_2A2


+CHEM--------RADJRAT
+COLPIVOT
+FLUSH
+FASTRATE
+FASTJAC
+FLUSH
+IRR_RATE
+COLPIVOT
+DEVCON
+SWITCH
+INITLZ----DEVCON
+PUFFDMP-----DELTAZ
+GETPT-------CALTOJ
+INTRVL
+HEDPTS
+UPDATE------JTOCAL
+CALTOJ
+RDFWND
+INTRVL
+HTFAGE
+FGRTRP
+RDFZP
+FFGTRP------REDUCR
+RDFRN
+RDFTMP
+GETBC-------CALTOJ
+INTRVL
+CNVTBC
+GETHAZ------CALTOJ
+INTRVL
+LFTPAK
+LFTPAK
+RDFKV
+RDFCLD
+RDFH2O
+CONVRT
+BEH084------FLUSH
+DIFFUS
+DIAGN-------CHKDAT
+FLUSH
+CKHGT
+HDRCHK
+RVMMAP------INTRVL
+ENDIND
+GUNIT-------JTOCAL
+ZELLAR
+GETQAR------CALTOJ
+INTRVL
+HEDQAR
+EFTOT
+PRINTR------JTOCAL
+NDAYSUB
+CALTOJ
+FGAVWR
+FGWRIT
+GXYWR
+FLUSH
+PGWRIT------PIGDMP------FLUSH
+DMPPIG
+FLUSH
+XCMPRT
+FCMPRT
+CUMPRT

4. MODEL INPUT REQUIREMENTS

In this section the content and format of the UAM-V simulation control file and each of the required data input files are described in detail.

UAM-V Command Line

The UAM-V command line on a Unix-like system takes the form

```
/path/uam-v run.in nn
```

where "path" specifies the directory in which the executable is stored, "uam-v" is the name of the executable file itself, "run.in" is the control file, and "nn" is an integer value controlling the level of program status information to be printed. If nn is omitted, it defaults to zero.

The value of the program status variable "nn" directs certain subroutines in the model to print additional status messages beyond the basic run-trace prints, which are always included during the course of a simulation. If a value of 0 is specified, only the basic run-trace messages are printed. A binary representation of the integer values is used in order to simplify the command line input and the computer code needed to interpret this information. Using the binary system, each routine is identified by a number, which is a power of 2, and a bit value. This enables a user to request messages from one or more routines by specifying one integer value that is either the value that corresponds to a specific routine or the sum of values for several routines. For example, using a value of 33 for the program status variable directs the model to print messages from both the main routine (value is 1) and the routine SETUP (value is 32). The bits currently used and the subroutines for which messages may be selected are listed in Table 4-1. The UAM-V converts the program status value internally and determines which bits are on or off (i.e., which routines should print status messages). Note that the basic runtime messages are quite adequate for most applications and that caution should be used in selection of additional messages as some routines generate copious amounts of output. A short run is advisable to determine if the messages will serve the required purpose and to estimate the volume of data produced. Most messages write to the command output file, but some also write to the simulation trace output file.

UAM-V Control File

The control file contains the pathnames of all other files to be read or written by the model and includes initialization and termination times for the simulation, options for the simulation, and a few data items that are not specified in other data files.

Table 4-1.
UAM-V program status variables.

Bit	Value	Subroutine	Purpose of routine; summary of messages
1	1	AAAMAIN	Main UAM-V routine; messages indicate when subroutines are called and total mass before and after certain steps of simulation.
2	2	FGRTRP	Interpolates data from coarse grid to fine grid; messages printed selected values before and after interpolation.
3	4	FSTEP	Selects size of advection steps for nested grids; messages indicate selected time step size.
4	8	RVMMAP	Reads aggregation file and sets parameters for grid nesting; messages print results of calculations during determination of grid nesting.
5	16	RCHEMF	Overall controller for chemistry calculations on nested grids; messages print data and concentrations before and after chemistry for selected grid cells.
6	32	SETUP	Opens files and performs initial reads from data files; messages indicate status of steps in the initialization process.
7	64	EMFINE	Adds emissions into fine-grid cells during a time step; messages indicate change in concentration due to emissions for selected cells.
8	128	STEPY	Advection in y-direction and z-direction on coarse grid; messages give concentrations before and after vertical advection at selected grid cells.
9	256	RCHEM	Overall controller for chemistry calculations on coarse grid; messages print data and concentrations before and after chemistry for selected grid cells.
10	512	CRSFIL	Fills a portion of coarse grid with concentrations from overlapping nested grid. Messages give concentrations before and after fill and cell parameters used in calculation for 1 grid cell only.
11	1024	EMCORS	Adds emissions into coarse grid cells during a time step; messages indicate change in concentration due to emissions for selected cells.
12	2048	CHREAD	Reads chemistry parameters file that specifies species to be simulated and reaction rates for chemical mechanism; messages indicate progress through routine and print values of certain parameters.
13	4096	UPDATE	Reads revised met data at specified intervals; messages print progress in updating data and results of certain calculations such as plume rise.
14	8192	TTRAJ	Controller routine for PiG treatment. Messages track many steps in plume history including location, width, dumping, and chemistry, for all puffs.
15	16384	XMSCAL, XMSPRT, XCMPRT	Diagnostic routines track flux from coarse grid to fine grid. Produces tables in diag file of fluxes across fine-grid boundaries based on coarse-grid variables. (For comparison with tables based on fine-grid variables.)

The content of the control file is described in detail in Tables 4-2 and 4-3. An example of the control file is shown in Exhibit 4-1. The control file begins with a list of model output files. The content of these files is described in Chapter 5. Following several lines describing the modeling domain, time span of the simulation, and simulation options, a line specifying the unit number and name of the Process Analysis (PA) control file is included. If the unit number is 0, then process analysis output will not be produced by the model. If the unit number is greater than zero, then a PA control file must be included. For further detail on the content of the PA control file, the reader is referred to the appendix.

The remainder of the UAM-V control primarily specifies the names of all input data files to be used in the simulation. Note that “restart files,” that is files from an earlier simulation from which a continuation simulation is being made, are included at the end of the control file.

In Table 4-2, lines that may be left out of the control file under certain conditions are shaded. (For instance, the line specifying the PiG parameters is left out when the PiG flag is false.) The condition under which the line must be included is defined under the column labeled "Selected by". There may also be entries in this column that do not apply to an entire line; certain data values or data file names may not be used by the UAM-V for some set of options. Space for these items must still be allocated on the input line. (For instance, if no fine grid temperature file is being used, the line specifying the fine grid temperature file name may begin with a unit number of 0. In this case, the filename of /dev/null will not be used by the model.) These items are underlined, and the condition that requires that they have valid information is listed in the "Selected by" column and is underlined.

The fine-grid domains (see lines 13 and 14 in Table 4-2) may be defined anywhere within the coarse grid with some restrictions. Fine-grid regions must be rectangles and must use the same number of subdivisions throughout a given fine grid. No cell aggregation is allowed on the fine grids. When fine grids are multiply nested (i.e., nests within nests), the factors in the control file refer to the ratio of the horizontal coarse-grid cell size to the horizontal fine-grid cell size. Fine-grid cell sizes are determined simply by dividing the coarse-grid cell size by the appropriate factor. For example, if the coarse-grid cell size is 10 km and the fine-grid factor (NHF in the control file) is 2, then the nested grid has cell size of 5 km.

The number of cells in a fine grid is determined by counting the number of coarse-grid cells to be subdivided, multiplying by the appropriate factor, and adding 2 to each dimension. If a 4-by-2 block of coarse-grid cells is subdivided into 5 km cells, the factor is 2, and the number of cells in the fine-grid data files is 10 by 6. Two cells are added to each dimension because of the way boundary cells are treated in the advection scheme. Concentrations are not calculated for these boundary cells, but space is allocated for them in memory by the model. In addition, data files must include values in these cells. Output files also include values in these cells, but they should not be used in any analyses.

Table 4-2.
UAM-V control file contents and format

Line	Contents	Format	Selected by
12	IERRLG, FNERRIOUT1(=66), FNOUT	I2,AI2,A	
3	IOUT2(=8), FNDIAG	I2,A	
4	IUAVG. ~~FNAVG~~	I2.A	~~IUAVG > 0~~
5	NAVSPC. (MAVSPC(L).L=1.NAVSPC)	I2.6A10./.(2X. 6A10)	IUAVG > 0
6	IINST(=51), FNINST	I2,A	
7	IFAVG, ~~FNFAVG~~	I2,A	~~IFAVG > 0~~
8	IFINST, ~~FNFINT~~	I2,A	~~IFINST > 0~~
9	IUPIGO, ~~FNPIG1~~	I2,A	~~IUPIGO > 0~~
10	~~IUPIGN~~, ~~FNPIG2~~	I2,A	~~IUPIGO > 0~~
11	IUO3, ~~FNO3~~	I2, A	~~IUO3 > 0~~
12	IPACRS, ~~FNPACRS~~	I2, A	~~IPACRS > 0~~
13	IPAFIN, ~~FNPAFIN~~	I2, A	~~IPAFIN > 0~~
13	MSG	A80	
14	TSTR, IDYSTR, TEND, IDYNF, DTDATA, DTPRNT, DTSTEP, DTAVG	*(free format)	
15	DLONG, DLAT, NOX, NOY, NLAYER, NOSPEC	2F7.0,4I5	
16	NUMFIN	I10	
17	(IXFB(IFINE). JYFB(IFINE).IXFE(IFINE). JYFE(IFINE).NHF(IFINE). NFZ(IFINE). IFINE=1. NUMFIN)	6I5	NUMFIN > 0
18	LWET, LRSTRT, LDEPN, LPIG, LCART, LINERT	6L10	
19	LAREA, LPTS, L1EDAY, LCHFAST	4L10	
20	L1DAY. LCHMAG. ISMTH. LSTAGR	2L10.I10.L10	
21	NRCLLS. WDUMP. XCMBN. DELPUF. DELOUT. MAXAGE	I2.2F10.2.3F10.0	LPIG = .TRUE.
22	DIFCOF, DIFMAX, DIFMIN, CHMINT	4F10.0	
23	WLONG, ELONG, SLAT, NLAT, TZ, UTMZON	4F10.2,F10.0,I10	
24	XORG, YORG	2F10.0	
25	PKRCHM, CRCHEM, LCHEM	2E10.2,L10	
26	IPAIN, FNPAIN	I2,A	
27	JCHEM, FNCHEM	I2,A	
28	MDF, FNMDF	I2,A	
29	MIXHT, FNMIX	I2,A	
30	ITEMP, FNTEMP	I2,A	
31	IUH2O, FNH2O	I2,A	
32	ISURF, FNSURF	I2,A	
33	EDF, FNEDF	I2,A	
34	AEM1, FNAEM1	I2,A	
35	AEM2, ~~FNAEM2~~	I2,A	~~AEM2 > 0~~
36	AEM3, ~~FNAEM3~~	I2,A	~~AEM3 > 0~~

Line	Contents	Format	Selected by
37	ICBC, ~~ENIC~~	I2,A	ICBC > 0
38	ICLOUD, ~~ENCLOUD~~	I2,A	~~ICLOUD > 0~~
39	IRAIN, ~~ENRAIN~~	I2,A	~~IRAIN > 0~~
40	ITERR, FNTERR	I2,A	
41	IKV, FNKV	I2,A	
42	~~DTMIN~~, ~~MAXITR~~, ~~RERROR~~	F10.0,I10,F10.0	~~LCHEM = .TRUE. & LINERT = .FALSE.~~
43	IAGG. FNAGG	I2.A	LCHMAG = .TRUE.
44	(IFMDF(I).~~ENFMDF~~.I=1.NUMFIN)	I2.A	NUMFIN > 0. ~~IFMDF(I) > 0~~
45	(IFKV(I).~~ENFKV~~.I=1.NUMFIN)	I2.A	NUMFIN > 0. ~~IFKV(I) > 0~~
46	(IFZP(I).~~ENZP~~.I=1.NUMFIN)	I2.A	NUMFIN > 0.~~IFZP(I) > 0~~
47	(IFTEMP(I).FNFTEMP.I=1.NUMFIN)	I2.A	NUMFIN > 0~~IFTEMP(I)~~ > 0
48	(IFUH2O(I).FNFH2O.I=1.NUMFIN)	I2.A	NUMFIN > 0~~IFUH2O(I)~~ > 0
49	(IFRAIN(I).FNFRAIN.I=1.NUMFIN)	I2.A	NUMFIN > 0~~IFRAIN(I)~~ > 0
50	(IFCLD(I).FNFCLD.I=1.NUMFIN)	I2.A	NUMFIN > 0~~IFCLD(I)~~ > 0
51	(IFSURF(I).FNFSURF.I=1.NUMFIN)	I2.A	NUMFIN > 0~~IFSURF(I)~~ > 0
	Read NUMFIN sets of the following three lines if NUMFIN > 0		
52	IFAEM1(I). FNFAEM1	I2.A	NUMFIN > 0
53	IFAEM2(I). ~~FNFAEM2~~	I2.A	NUMFIN > 0. ~~IFAEM2(I) > 0~~
54	IFAEM3(I). ~~FNFAEM3~~	I2.A	NUMFIN > 0. ~~IFAEM3(I) > 0~~
51	NPHVAL. FNPH	I2.A	LINERT = .FALSE.
50	NPHVAL, FNAHO	I2,A	LINERT = .FALSE.
51	ICBC, FNTOPC	I2,A	
52	ICBC, FNBNDC	I2,A	
53	IDEP. ~~FNDEP~~	I2.A	~~IDEP > 0~~
54	IPIG. ~~FNPIGDMP~~	I2.A	~~IPIG >0~~and LPIG = .TRUE.
55	FNCONC (opened on unit 98)	A	LRSTRT = .TRUE.
56	FNFCONC (opened on unit 99)	A	LRSTRT = .TRUE. and NUMFIN > 0
57	FNPIG (opened on unit 97)	A	LRSTRT = .TRUE. and LPIG = .TRUE.

Table 4-3.
UAM-V control file variable names

Variables	Definition	Data Type
IERRLG	Unit number for UAM-V error log file. Typical value is 14.	Integer
FNERR	Name of UAM-V error log file	Char*80
IOUT1	= 66, Unit number of UAM-V output information file (SIMOUT)	Integer
FNOUT	Name of UAM-V (formatted) output information file showing program control (SIMOUT)	Char*80
IOUT2	= 8, Unit number of UAM-V diagnostic output file (DIAG)	Integer
FNDIAG	Name of UAM-V (formatted) diagnostic output file (DIAG)	Char*80
IUAVG	Unit number of coarse-grid average concentration file	Integer
FNAVG	Name of (unformatted) coarse-grid hourly first-layer average concentration file; opened only when IUAVG > 0	Char*80
NAVSPC	Number of species to be output for average concentrations	Integer
MAVSPC(L)	Name of each species L to be output for average concentrations. Note: the 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 files.)	Char*10
IINST	= 51, Unit number of coarse-grid instantaneous concentration file	Integer
FNINST	Name of (unformatted) coarse-grid instantaneous concentration file	Char*80
IFAVG	Unit number of fine-grid average concentration file	Integer
FNFAVG	Name of (unformatted) fine-grid hourly 1st-layer average concentration file; opened only when IFAVG > 0	Char*80
IFINST	Unit number of fine-grid instantaneous concentration file	Integer
FNFINT	Name of (unformatted) fine-grid instantaneous concentration file; opened only when IFINST > 0	Char*80
IUPIGO	Unit number of PiG restart file 1	Integer
FNPIG1	Name of (unformatted) PiG output file 1 for future restart; opened only when IUPIGO > 0	Char*80
IUPIGN	Unit number of PiG restart file 2	Integer
FNPIG2	Name of (unformatted) PiG output file 2 for future restart; opened only when IUPIGN > 0	Char*80
IUO3	Unit number of step-by-step ozone output file	Integer
FNO3	Name of (unformatted) step-by-step ozone file; opened only when IUO3 > 0	Char*80
IPACRS	Unit number of coarse grid process analysis output file (must be = 3 if process analysis output is desired or 0 otherwise)	Integer
FNPACRS	Name of (unformatted) coarse grid process analysis output file; opened only when IPACRS > 0	Char*80
IPAFIN	Unit number of fine grid process analysis output file (must be = 4 if process analysis output is desired for fine grids or 0 otherwise)	Integer
FNPAFIN	Name of (unformatted) fine grid process analysis output file; opened only when IPAFIN > 0	Char*80
MSG	Message or UAM-V run title	Char*80

Variables	Definition	Data Type
TSTR	Time at which the simulation is to begin; military hour, ex. 900.0 is 9 a.m.	Real
IDYSTR	Date on which simulation is to begin, optionally calendar (YYMMDD or YYYYMMDD) or Julian (YYDDD) format; ex. February 3, 1990 is 900203 or 90034. Calendar dates in year 2000 or later must use 4 digit years (e.g., 20000101 is January 1, 2000).	Integer
TEND	Time at which simulation is to terminate; military hour	Real
IDYNF	Date on which simulation is to terminate (YYMMDD, YYYYMMDD, or YYDDD)	Integer
DTDATA	Input meteorological data update interval, in military hour (i.e., 100. = 1 hour interval). Typical value is 100.	Real
DTPRNT	Concentration output interval, in military hour. Typical value is 100.	Real
DTSTEP	Maximum time step for advection calculation, in minutes. Typical value is 15.	Real
DTAVG	Minimum interval for calculation of rolling average O3. Typical value is 1.	Real
DLONG	East-west grid spacing, in degrees longitude if latitude/longitude coordinates are chosen; otherwise in km when Cartesian coordinates are used. (See LCART below.)	Real
DLAT	North-south grid spacing, in degrees latitude or in km	Real
NOX	Number of coarse-grid cells in the east-west direction	Integer
NOY	Number of coarse-grid cells in the north-south direction	Integer
NLAYER	Number of coarse-grid vertical layers	Integer
NOSPEC	Number of chemical species	Integer
NUMFIN	Number of fine ("nested") grids	Integer
IXFB(IFINE),JYFB(IFINE)	Lower left (SW) coarse grid cell covered by fine grid number IFINE.	Integer
IXFE(IFINE),JYFE(IFINE)	Upper right (NE) coarse grid cell covered by fine grid number IFINE.	Integer
NHF(IFINE)	Number of horizontal subdivisions along one dimension of coarse grid cells to match resolution of fine 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).	Integer
NZF(IFINE)	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.	Integer
LWET	if LWET = .TRUE. wet deposition calculations are made during the simulation. A rainfall rate data file is required.	Logical
LRSTRT	if = .TRUE., this is a restart of a previous run and restart files are required to reinitialize the model. (See FNCONC, FNFCONC and FNPIG below.)	Logical
LDEPN	if = .TRUE. dry deposition calculations are made during the simulation	Logical
LPIG	if = .TRUE., selected point sources are handled by the sub-grid scale Plume-in Grid treatment	Logical
LCART	= .TRUE., when Cartesian coordinates are used (km);= .FALSE., when lat/long coordinates (in degrees) are used.	Logical
LINERT	if = .TRUE., no photochemical calculations are made	Logical
LAREA	if = .TRUE., area source emissions are included in simulation	Logical

Variables	Definition	Data Type
LPTS	if = .TRUE., elevated point sources are included in simulation	Logical
L1EDAY	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.	Logical
LCHFAST	if = .TRUE., use the fast chemistry solver for solving chemistry step which results in execution times approximately 4 times less than the standard solver, but makes some approximations in the solution for fast reacting species. if = .FALSE., use standard chemistry solver.	Logical
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	Logical
LCHMAG	if = .TRUE., a file is required defining grid cells to be aggregated for chemistry calculation purposes	Logical
ISMTH	defines smoothing technique to be used in chemistry aggregation: = 1, calculated mass in aggregated cell is distributed to constituent cells according to a "gradient-conserving" technique.= 2, mass in aggregated cell is distributed to constituent cells according to mass ratios among cells before aggregation calculation. This is the recommended and default value.= 3, mass in aggregated cell is distributed to composing cells homogeneously.	Integer
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.	Logical
NRCLLS	Number of elliptical layers (or "skins") of each plume treated with PiG. Recommended value is 4.	Integer
WDUMP	Factor to be multiplied with the cross-sectional area of the plume to be compared with the (vertical) cross-sectional area of a grid cell before dumping a skin of the plume into that grid cell. A value less than or equal to 1.0 is recommended.	Real
XCMBN	Maximum horizontal distances (km) of different sources with the same stack height to be combined as one plume. Recommended value is 0.1 km.	Real
DELPUF	Time interval between puff releases (min). Recommend that the value be as small or smaller than a coarse-grid time step.	Real
DELOUT	Time interval between PiG outputs (min). Recommended value is 60 min.	Real
MAXAGE	Maximum lifetime of a plume (hours). After this time, the plume is dumped into the grid. Recommended value is 24 hrs.	Real
DIFCOF	Empirical parameter for horizontal diffusion coefficient, in min^{-1}. Default value (= 0.25/≤ 2) is used when DIFCOF ≤ 0.0.	Real
DIFMAX	Maximum horizontal diffusivity, in km^2/min. Default value (= 0.6) is used when DIFMAX ≤ 0.0.	Real
DIFMIN	Minimum horizontal diffusivity, in km^2/min. Default value (= 0.0006) is used when DIFMIN ≤ 0.0.	Real
CHMINT	Factor to multiply by advection time step to get chemistry integration step when chemistry aggregation is applied. Not used when LCHMAG = .FALSE.; must be < 2.0 when LCHMAG = .TRUE. Recommended value is 1.0.	Real

Variables	Definition	Data Type
WLONG	Longitude of west boundary of modeling region (negative value in western hemisphere), in degrees	Real
ELONG	Longitude of east boundary of modeling region, in degrees	Real
SLAT	Latitude of south boundary of modeling region, in degrees	Real
NLAT	Latitude of north boundary of modeling region, in degrees	Real
TZ	Time zone (5.0 = EST; 6.0 = CST; 7.0 = MST; 8.0 = PST; 0.0 = GMT)	Real
UTMZON	UTM zone number of the modeling domain (should be negative or 0 if a coordinate system other than UTM is being used.)	Integer
XORG	X coordinate of the origin (i.e. lower-left corner) of the modeling domain, in UTM km (or km in another Cartesian coordinate system); it is a dummy variable if LCART = .FALSE.	Real
YORG	Y coordinate of the origin of the modeling domain, in UTM km (or km in another Cartesian system), it is a dummy variable if LCART = .FALSE.	Real
PKRCHM	Peak diurnal photochemical reaction rate for SO_2 and NOx, in min^{-1}, used only when LCHEM = .FALSE. Recommended value is $3.333 \leq 10^{-4}$.	Real
CRCHEM	Minimum diurnal photochemical reaction rate for conversion of SO_2 to SO_4, in min^{-1}, used only when LCHEM = .FALSE. Recommended value is $8.333 \leq 10^{-5}$.	Real
LCHEM	if = .FALSE., linear (SO_2/SO_4) chemistry is simulated;if = .TRUE., full oxidant chemistry is simulated	Logical
IPAIN	Unit number of process analysis control file (must be 2 if process analysis is to be used or 0 otherwise)	Integer
FNPAIN	Name of (formatted) process analysis control file (See Appendix 1 for detailed information on formats and options.)	
JCHEM	Unit number of chemical mechanism specification file	Integer
FNCHEM	Name of (formatted) chemical mechanism specification file, which includes species names, reaction rate constants, etc.	Char*80
MDF	Unit number of wind data file (WIND)	Integer
FNMDF	Name of (unformatted) wind data file (WIND)	Char*80
MIXHT	Unit number of file containing vertical layer heights (HEIGHT)	Integer
FNMIX	Name of (unformatted) file containing vertical layer heights (HEIGHT)	Char*80
ITEMP	Unit number of temperature file (TEMPERATURE)	Integer
FNTEMP	Name of (unformatted) temperature file (TEMPERATURE)	Char*80
IUH2O	Unit number of file containing water vapor concentrations (H2O)	Integer
FNH2O	Name of (unformatted) water vapor concentration file (H2O)	Char*80
ISURF	Unit number of file containing surface-cover types (SURFACE)	Integer
FNSURF	Name of (unformatted) surface-cover type file (SURFACE)	Char*80
EDF	Unit number of elevated point source stack specification and emission data file (PTSOURCE)	Integer
FNEDF	Name of (formatted) elevated point source stack specification and emission data file (PTSOURCE)	Char*80
AEM1	Unit number of weekday area source emission file (EMISSIONS)	Integer
FNAEM1	Name of (unformatted) weekday area source emission file (EMISSIONS)	Char*80

Variables	Definition	Data Type
AEM2	Unit number of Saturday area source emission file (EMISSIONS)	Integer
FNAEM2	Name of (unformatted) Saturday area source emission file (EMISSIONS); opened only when AEM2 > 0	Char*80
AEM3	Unit number of Sunday area source emission file (EMISSIONS)	Integer
FNAEM3	Name of (unformatted) Sunday area source emission file (EMISSIONS); opened only when AEM3 > 0	Char*80
ICBC	Unit number of initial concentration file (AIRQUALITY)	Integer
FNIC	Name of (unformatted) initial concentration data file (AIRQUALITY) (Use /dev/null if LRSTRT = .TRUE.)	Char*80
ICLOUD	Unit number of cloud characteristics file (CLOUD)	Integer
FNCLOUD	Name of (unformatted) cloud characteristics file (CLOUD)	Char*80
IRAIN	Unit number of rainfall rate data file (RAIN)	Integer
FNRAIN	Name of (unformatted) rainfall rate data file (RAIN)	Char*80
ITERR	Unit number of terrain height data file (TERRAIN)	Integer
FNTERR	Name of (unformatted) terrain height data file (TERRAIN)	Char*80
IKV	Unit number of vertical diffusivity file (VDIFFUSION)	Integer
FNKV	Name of (unformatted) vertical diffusivity file (VDIFFUSION)	Char*80
DTMIN	Minimum allowable time step for chemistry integration, in hours. Recommended value is 0.00001.	Real
MAXITR	Maximum number of iterations for chemistry integration. Recommended value is 5.	Integer
RERROR	Relative error tolerance for chemistry integration. Recommended value is 0.02.	Real
IAGG	Unit number of file defining chemistry aggregation and grid nesting (AGGMAP)	Integer
FNAGG	Name of (formatted) file defining chemistry aggregation (AGGMAP)	Char*80
IFMDF(I)	Unit number of wind data file for the *i*th fine grid domain	Integer
FNFMDF	Name of (unformatted) wind data file for the *i*th fine grid domain; opened only when IFMDF(I) > 0	Char*80
IFKV(I)	Unit number of vertical diffusivity data file for the *i*th fine grid domain	Integer
FNFKV	Name of (unformatted) vertical diffusivity file for the *i*th fine grid domain; opened only when IFKV(I) > 0	Char*80
IFZP(I)	Unit number of height/pressure data file for *i*th fine-grid domain	Integer
FNZP	Name of (unformatted) height/pressure data file for *i*th fine-grid domain; opened only when ISZP(I) > 0	Char*80
IFTEMP(I)	Unit number of temperature data file for the *i*th fine-grid domain	Integer
FNFTEMP	Name of (unformatted) temperature data file for the *i*th fine-grid domain	Char*80
IFUH2O(I)	Unit number of water vapor data file for the *i*th fine-grid domain	Integer
FNFH2O	Name of (unformatted) water vapor data file for the *i*th fine-grid domain	Char*80
IFRAIN(I)	Unit number of rain data file for the *i*th fine-grid domain	Integer
FNFRAIN	Name of (unformatted) rain data file for the *i*th fine-grid domain	Char*80
IFCLD(I)	Unit number of cloud data file for the *i*th fine-grid domain	Integer

Variables	Definition	Data Type
FNFCLD	Name of (unformatted) cloud data file for the *i*th fine-grid domain	Char*80
IFSURF(I)	Unit number of surface data file for the *i*th fine-grid domain	Integer
FNFSURF	Name of (unformatted) surface data file for the *i*th fine-grid domain	Char*80
IFAEM1(I)	Unit number of weekday area emission data file for the *i*th fine grid domain	Integer
FNFAEM1	Name of (unformatted) weekday area emission data file for the *i*th fine grid domain; opened only when IFAEM1(I) > 0	Char*80
IFAEM2(I)	Unit number of Saturday area emission data file for the *i*th fine grid domain	Integer
FNFAEM2	Name of (unformatted) Saturday area emission data file for the *i*th fine grid domain; opened only when IFAEM2(I) > 0	Char*80
IFAEM3(I)	Unit number of Sunday area emission data file for the *i*th fine grid domain	Integer
FNFAEM3	Name of (formatted) Sunday area emission data file for the *i*th fine grid domain; opened only when IFAEM3(I) > 0	Char*80
NPHVAL	Unit number of data file containing photolysis rates as functions of zenith angle and height	Integer
FNPH	File name of formatted data file containing photolysis rates of no2, hchor, hchos, o3o1d, alds, and acrolein	Char*80
NPHVAL	Unit number of ALBEDO/HAZE/OZONE COL file	Integer
FNAHO	File name of formatted ALBEDO/HAZE/OZONE COL file	Char*80
ICBC	Unit number of aloft concentration data file (TOPCONC)	Integer
FNTOPC	File name of formatted aloft concentration data file (TOPCONC)	Char*80
ICBC	Unit number of coarse-grid boundary concentration data file(BOUNDARY)	Integer
FNBNDC	File name of (unformatted) coarse-grid boundary concentration data file (BOUNDARY)	Char*80
IDEP	Unit number of coarse-grid deposition file (normally IDEP=0, in which case the data file is not read and deposition rates are calculated internally)	Integer
FNDEP	File name of (unformatted) coarse-grid deposition file. (May be /dev/null if IDEP=0)	Char*80
IPIG	Unit number of P-i-G dump file; if IPIG=0, no P-i-G dump file is written	Integer
FNPIGDMP	File name of (unformatted) P-i-G dump file (May be /dev/null if IPIG=0)	Char*80
FNCONC	File name of (unformatted) coarse-grid instantaneous concentrations data file from the previous run, opened on unit number 98. Used for restarts.	Char*80
FNFCONC	File name of (unformatted) fine grid instantaneous concentrations data file from the previous run, opened on unit number 99. Used for restarts.	Char*80
FNPIG	File name of (unformatted) PiG restart file from the previous run, opened on unit 97.	Char*80

Exhibit 4-1.
Sample control file for UAM-V version 1.30

```
74/disk1/someplace/uamv/output/asc/err.cf.13sep97.SOMEPLACE-9.97-97-0.00
66/disk1/someplace/uamv/output/asc/simu.cf.13sep97.SOMEPLACE-9.97-97-0.00
08/disk1/someplace/uamv/output/asc/diag.cf.13sep97.SOMEPLACE-9.97-97-0.00
61/disk1/someplace/uamv/output/bin/avrg.cc.13sep97.SOMEPLACE-9.97-97-0.00
24NO        NO2       O3        OLE       PAR       TOL
  XYL       HCHO      ACET      ETH       PAN       CO
  HNO2      HNO3      ISOP      ETOH      MEOH      ISPD
  PANX      IOLE      ALDX      CRES      PACET     PHCHO
51/disk1/someplace/uamv/output/bin/inst.cc.13sep97.SOMEPLACE-9.97-97-0.00
62/disk1/someplace/uamv/output/bin/avrg.ff.13sep97.SOMEPLACE-9.97-97-0.00
52/disk1/someplace/uamv/output/bin/inst.ff.13sep97.SOMEPLACE-9.97-97-0.00
71/disk1/someplace/uamv/output/bin/pig1.13sep97.SOMEPLACE-9.97-97-0.00
72/disk1/someplace/uamv/output/bin/pig2.13sep97.SOMEPLACE-9.97-97-0.00
00/dev/null
03/disk1/someplace/uamv/output/bin/pa.cc.13.Run00
04/disk1/someplace/uamv/output/bin/pa.ff.13.Run00
UAMV 1.17: SOMEPLACE 13sep97 SOMEPLACE-9.97-97-0.00
 0000.0 970913 0000.0 970914  100.0  100.0   15.0     1.
    0.5 .33333   49   38    8   29
5
 5    6   35   29   3    8
26   22   30   27   9    8
21   22   25   26   9    8
 9   10   27   17   9    8
13   13   15   16   18   8
true      true      true      true      false     false
true      true      true      true
false     false        2      false
 4      0.50     0.001      30.0     240.0       12.
00.00     0.60      0.0006    1.0
    -98.00    -73.50     25.67     38.33        5.        -9
-98.0     25.6667
3.333E-4  8.333E-5  true
02pa.cf.run00.in
10/disk7/someplace/uamv/inputs/other/chempar1.17.in
12/disk7/someplace/uamv/inputs/met/grd1.wnd.970913.someplace
13/disk7/someplace/uamv/inputs/met/grd1.hgt.970913.someplace
14/disk7/someplace/uamv/inputs/met/grd1.tmp.970913.someplace
15/disk7/someplace/uamv/inputs/met/grd1.hum.970913.someplace
16/disk7/someplace/uamv/inputs/other/sfc.someplace_1.36km.bin
17/disk1/someplace/eps2/omef/ptsrce.r1.970913.someplace97.pig
18/disk6/someplace/eps2/omef/emiss.all.r1.970913.someplace97
00/dev/null
00/dev/null
39/dev/null
20/disk7/someplace/uamv/inputs/met/grd1.cld.970913.someplace
21/disk7/someplace/uamv/inputs/met/grd1.rain.970913.someplace
22/disk7/someplace/uamv/inputs/other/terr.someplace_1.dum
23/disk7/someplace/uamv/inputs/met/grd1.kvs.970913.someplace
0.00001            5      0.02
31/disk7/someplace/uamv/inputs/met/grd2.wnd.970913.someplace
32/disk7/someplace/uamv/inputs/met/grda.wnd.970913.someplace
33/disk7/someplace/uamv/inputs/met/grdb.wnd.970913.someplace
```

```
34/disk7/someplace/uamv/inputs/met/grdc.wnd.970913.someplace.a1
00/dev/null
35/disk7/someplace/uamv/inputs/met/grd2.kvs.970913.someplace
36/disk7/someplace/uamv/inputs/met/grda.kvs.970913.someplace
37/disk7/someplace/uamv/inputs/met/grdb.kvs.970913.someplace
38/disk7/someplace/uamv/inputs/met/grdc.kvs.970913.someplace.a1
00/dev/null
89/disk7/someplace/uamv/inputs/met/grd2.hgt.970913.someplace
40/disk7/someplace/uamv/inputs/met/grda.hgt.970913.someplace
41/disk7/someplace/uamv/inputs/met/grdb.hgt.970913.someplace
42/disk7/someplace/uamv/inputs/met/grdc.hgt.970913.someplace.a1
00/dev/null
43/disk7/someplace/uamv/inputs/met/grd2.tmp.970913.someplace
44/disk7/someplace/uamv/inputs/met/grda.tmp.970913.someplace
45/disk7/someplace/uamv/inputs/met/grdb.tmp.970913.someplace
46/disk7/someplace/uamv/inputs/met/grdc.tmp.970913.someplace.a1
00/dev/null
47/disk7/someplace/uamv/inputs/met/grd2.hum.970913.someplace
48/disk7/someplace/uamv/inputs/met/grda.hum.970913.someplace
49/disk7/someplace/uamv/inputs/met/grdb.hum.970913.someplace
50/disk7/someplace/uamv/inputs/met/grdc.hum.970913.someplace.a1
00/dev/null
53/disk7/someplace/uamv/inputs/met/grd2.rain.970913.someplace
54/disk7/someplace/uamv/inputs/met/grda.rain.970913.someplace
55/disk7/someplace/uamv/inputs/met/grdb.rain.970913.someplace
56/disk7/someplace/uamv/inputs/met/grdc.rain.970913.someplace.a1
00/dev/null
57/disk7/someplace/uamv/inputs/met/grd2.cld.970913.someplace
58/disk7/someplace/uamv/inputs/met/grda.cld.970913.someplace
59/disk7/someplace/uamv/inputs/met/grdb.cld.970913.someplace
60/disk7/someplace/uamv/inputs/met/grdc.cld.970913.someplace.a1
00/dev/null
63/disk7/someplace/uamv/inputs/other/sfc.someplace_2.12km.bin
64/disk7/someplace/uamv/inputs/other/sfc.someplace_a.4km.bin
65/disk7/someplace/uamv/inputs/other/sfc.someplace_b.4km.bin
67/disk7/someplace/uamv/inputs/other/sfc.someplace_c.4km.bin
00/dev/null
80/disk6/someplace/eps2/omef/emiss.all.r2.970913.someplace97
00/dev/null
00/dev/null
81/disk6/someplace/eps2/omef/emiss.all.rA.970913.someplace97
00/dev/null
00/dev/null
82/disk6/someplace/eps2/omef/emiss.all.rB.970913.someplace97
00/dev/null
00/dev/null
83/disk6/someplace/eps2/omef/emiss.all.rC.970913.someplace97
00/dev/null
00/dev/null
84/disk6/someplace/eps2/omef/emiss.all.rD.970913.someplace97
00/dev/null
00/dev/null
69/disk7/someplace/uamv/inputs/other/rate117.ng.970910-970918.someplace
69/disk7/someplace/uamv/inputs/other/albhzoz.cf.someplace.970910-970918
39/disk7/someplace/uamv/inputs/other/someplace_topcn.in
39/disk7/someplace/uamv/inputs/other/someplace_bndry.bin
```

```
00/dev/null
11/disk1/someplace/uamv/output/bin/pigd.13sep97.SOMEPLACE-9.97-97-0.00
/disk1/someplace/uamv/output/bin/inst.cc.12sep97.SOMEPLACE-9.97-97-0.00
/disk1/someplace/uamv/output/bin/inst.ff.12sep97.SOMEPLACE-9.97-97-0.00
/disk1/someplace/uamv/output/bin/pig1.12sep97.SOMEPLACE-9.97-97-0.00
```

Fine grids are numbered by the model as they are encountered during the definition process. It is occasionally useful to know the numbers assigned to the fine grids. They are printed on the diagnostic file in the summary of the fine-grid definition. The user can also deduce the numbers by numbering the fine-grid definition lines in the control file. Fine grids are numbered sequentially as they are encountered. The user must order the definition such that outer grids are defined prior to inner grids. As mentioned above, information about the size, location, and resolution of the main grid and nested grids as well as the number of vertical layers and vertical nesting instructions is specified in the control file. The vertical layer structure for each grid point must be specified in the HEIGHT file (see below) if the fine-grid layer structure differs from the coarse-grid structure. The optional chemical aggregation map file is also described below.

Standardized File Headers

Each of the meteorological input files for UAM-V version 1.30 includes a set of standardized header records. These header records identify the type of file and give some region definition information. Although the data in the headers is not used during a simulation, some of the information is checked against the region definition provided in the control file. Inconsistencies will result in warning messages. The files that include these standardized headers are the HEIGHT, TEMPERATUR, WIND, H2O, SURFACE, CLOUD, RAIN, VDIFFUSION, and TERRAIN files. The structure of the headers is the same for the coarse and fine grid files and is presented in Table 4-4.

Layer Height Definition (HEIGHT)

For each model layer at each horizontal grid location, the HEIGHT file defines (1) the height in meters above ground level (AGL) of the layer top and (2) the atmospheric pressure in millibars at the layer midpoint. Atmospheric pressure is used for the calculation of some chemical reaction rates. The HEIGHT file is typically derived from prognostic meteorological model output using various postprocessing procedures. Each of these quantities can vary in space and time; however, it is recommended that layer heights be temporally invariant.

This binary (unformatted) data file has a maximum record length of 2 plus NOX times NOY. The user is requested to provide data for the coarse grid only. Data are interpolated internally to the fine grid resolution from the coarse grid data if no fine-grid HEIGHT file is supplied. If vertical grid nesting is requested for a fine grid in the control file, the user must provide a height file for that fine grid. Fine grids may have more layers than the coarse grid, but not less. In addition, the top of every layer in the coarse grid must coincide with the top of some layer in the fine grid. The correspondence between layers in the coarse and fine grids must remain the same across space and time. For example, suppose that the coarse grid has five layers and the fine grid has six. If the additional fine-grid layer is located below the top of the coarse-grid layer 1, then the coarse-grid layer 1 height must be equal to the fine-grid layer 2 height. Furthermore, the coarse-grid layer 2 height must be equal to fine-grid layer 3 height and so forth to the top of the domain. At another location in the grid or later in the simulation, the additional fine-grid layer may not be moved above the coarse-grid layer 1.

Table 4-4.
Standardized headers records for UAM-V meteorological files

Record	Variable name	Variable type	Description

Record	Variable name	Variable type	Description
Record 1	filhdr	Character*10	Identifies the file type such as WIND or TEMPERATUR
	note	Character*80	A comment line which can contain any identifying text that the user wishes
Record 2	ivers	integer*4	A version identifier which will potentially allow us to update the format of files if future data requirements change. For now, this will always be zero.
	icoord	integer*4	To be used to identify the coordinate system used for defining the grid system (e.g., 0 for lat/lon, 1 for UTM, 2 for Lambert conformal grid, etc).
	nspec	integer*4	Number of species on file for files such as BOUNDARY or EMISSIONS. Zero for files such as TEMPERATUR which do not include species.
	idat	integer*4	Beginning date of data on file either as Julian (yyddd) date or as calendar date (yymmdd or yyyymmdd for year 2000 and beyond).
	timbeg	real*4	Beginning time of data on file in hours (e.g., 1:30 PM would be 13.5).
	iend	integer*4	End date of data on file
	timend	real*4	End time of data on file
Record 3	xorg	real*4	East-west (x) coordinate of origin of grid in units consistent with the coordinate system defined by icoord. (i.e., coordinate of southwest corner of grid cell 1,1 in lat/lon if icoord = 0, otherwise in km)
	yorg	real*4	North-south (y) coordinate of origin of grid.
	dx	real*4	Grid spacing in east-west direction in units consistent with icoord, either degrees or km.
	dy	real*4	Grid spacing in north-south direction in units consistent with icoord, either degrees or km.
	nx	integer*4	Number of grid cells in east west direction.
	ny	integer*4	Number of grid cells in north-south direction
	nz	integer*4	Number of verticals levels of data in grid.
	izone	integer*4	UTM zone number if using UTM coordinate system (zero otherwise).

The three standard header records appear at the beginning of the file. The following records then are repeated for each data interval:

Record 1: TIME, IDATE, ((HNEW(I,J),I=1,NOX),J=1,NOY)	| Repeat | NLAYER
Record 2: TIME, IDATE, ((PRESS(I,J),I=1,NOX),J=1,NOY)	| times

This group of records is repeated as necessary to cover the time span of the simulation at the interval specified in the control file, plus one extra hour for interpolation. (That is, a 24-hour simulation requires 25 intervals of data.)

TIME is a real number representing military time (e.g., 2300. = 11:00 PM) or hours (e.g., 23.0 = 11:00 PM). IDATE is an integer representing the date either as a calendar date (YYMMDD or YYYYMMDD for year 2000 and beyond) or a Julian style date (YYDDD). The model uses the height data that follow at the date and time indicated and reads the next interval so that heights can be interpolated in time between data intervals. Since times and dates for HNEW and PRESS must match, the pressure is also read for the next interval. PRESS is not, however, interpolated. The TIME and IDATE variables on the PRESS record therefore specify that the pressure data are used up until that time. If the L1DAY flag in the control is true, the date is ignored and only the time is checked. HNEW is the height of the top of the cell in meters above ground; PRESS is atmospheric pressure in millibars at the center of the cell.

Chemical Aggregation (AGGMAP)

This is an optional file that defines the locations of coarse grid cells to be aggregated for chemistry calculations. Aggregation reduces the computation time required to solve the chemistry, and may be used where the spatial variability of species concentrations is expected to be small. If four cells are aggregated into one, for example, then chemistry calculations are eliminated for three cells. Ideally, test simulations should be made to verify that the aggregation used does not significantly alter model results.

The AGGMAP file consists of maps in which each coarse grid cell is represented by a single character. The maps therefore are NOY rows of NOX characters each. The top row corresponds to North (i.e., J=NOY) and the bottom corresponds to South (J=1). Aggregation may be changed at hourly intervals. Further details of the format of the aggregation map file are presented in Table 4-5.

A map consisting of a set of two-dimensional integer arrays (each member of the set is one layer) indicates clusters of grid cells to be treated as aggregate cells for chemistry calculations. Aggregation is allowed only on coarse-grid cells that are not overlapped by any nested fine grids. The three-dimensional aggregate cells must be characterizable by three orthogonal lengths representing multiples of the fundamental (i.e., smallest) grid dimensions, although the user need not specify these. They are determined automatically. The user must provide one "map" for each layer. Each map consists of aggregate cells suitably "colored" by one-character integers. Allowable "colors" are 1 through 9.

Table 4-5.
Format of UAM-V aggregation map file (AGGMAP)

Repeat Count	Content of Line	Format	Description of Data
Repeat following group of lines for K = 1 through NLAYER			

Repeat Count	Content of Line	Format	Description of Data
Repeat following group of lines for K = 1 through NLAYER			
1 line	IVTIME, IVDAY	I4, 1X, I6	Time and date at which the following aggregation map will begin to be used. Time is military time (e.g., 1400 is 2:00 p.m.). Date must match the date used in defining the span of the simulation in the control file, whether Julian (YYDDD) or calendar (YYMMDD).
NOY lines	(IVMM(I,J,K),I=1,NOX)	80I1	Array of "color" codes, integers from 0 to 9. First line is for top (north) row in region (J=NOY) progressing to bottom (south) row (J=1). One code for each grid cell. Contiguous cells with like codes are aggregated for chemistry purposes. Value 0 designates a boundary cell not included in the simulation; 9 means that the cell is not to be included in any aggregate. See text for further discussion.

Boundary cells must be "colored" with the integer 0. Boundaries may be irregular. For example, the following map contains 32 aggregate cells in a particular layer (5 of which are clusters of cells).

0000000000000000

0111113332212430

0111113331341210

0111112213121400

0444442231213000

0444441412120000

0000000000000000

The aggregates are:

- One 5 $\times$ 3 cell in the upper left corner.
- One 5 $\times$ 2 cell in the lower left corner.
- One 3 $\times$ 2 cell in the upper middle.
- One 2 $\times$ 1 cell to the right of the previous one.
- One 2 $\times$ 2 cell just left and below the center.
- 27 one-cell aggregates.

Note that all other fundamental cells (the one-cell aggregates) are identified with integers unique with respect to adjacent cells (recall the four-color map problem). When "coloring" the adjacent layer, make sure no vertically adjacent cells are colored the same unless they form part of an aggregate. For example, the following map for layer 2 would aggregate the upper left-hand cluster of cells in layer 1 with layer 2:

0000000000000000

0111115656565650

0111116565656560

0111115656565650

0565656565656560

0656565656565650

0000000000000000

Unintentional vertical aggregation can be avoided by using the integers 1–4 and 5–8 for alternating model layers. The model checks that vertical aggregation is specified properly. For example, identifying a 5 $\times$ 2 block of cells in the upper left corner in layer 2 is invalid because the aggregate cannot be specified in terms of three ranges of grid indices.

One final note: Maps should be created with north along the upper row as on a map.

J indices are reversed by the model.

Geographic Inputs

Surface Characteristics (SURFACE)

The surface characteristics file contains the distribution of land-use types for each horizontal grid cell. Land-use type determines the UV albedo, roughness height, and surface resistance to deposition for gaseous species. Land-use inputs are generally extracted from the USGS land-use database. Surface characteristics may vary spatially but not temporally.

A SURFACE file is a binary (unformatted) data file with a maximum record length of NOX times NOY times MLUS (number of land-use categories). A SURFACE file must be provided for the

outer (coarse) grid in a nested-grid simulation. SURFACE files can optionally be inputted for fine-grid subdomains. If a fine-grid SURFACE file is not provided, data from the coarse-grid SURFACE file are interpolated to the fine grid. Following the three standard header records, the record structure of the file is as follows:

Record 1: (((FLAND(I,J,K),I=1,NOX),J=1,NOY),K=1,MLUS)

where FLAND is the fraction of land-use category K in each grid cell. Summing FLAND over all values of K within one grid cell should yield 1. MLUS is the number of categories employed by the UAM-V (currently 11). The land-use categories currently employed by the UAM-V and the roughness lengths associated with them are tabulated in Table 4-6.

Table 4-6.
Land-use categories recognized by UAM-V
Surface roughness and UV albedo values are given for each category.

Category Number	Land-Use Category	Surface Roughness (meters)	UV Albedo
1	Urban	3.00	0.08
2	Agricultural	0.25	0.05
3	Range	0.05	0.05
4	Deciduous forest	1.00	0.05
5	Coniferous forest including wetland	1.00	0.05
6	Mixed forest	1.00	0.05
7	Water	0.0001	0.04
8	Barren land	0.002	0.08
9	Nonforest wetlands	0.15	0.05
10	Mixed agricultural and range	0.10	0.05
11	Rocky (low shrubs)	0.10	0.05

Preprocessors are available to develop the surface file from USGS or other land-use data (PRELND or POSTLND, depending on the type of USGS data used). These preprocessors are described elsewhere.

Terrain Height Definition (TERRAIN)

This file defines the ground level altitude (above sea level) of each horizontal coarse grid location. Values of terrain heights are not currently used in UAM-V. All terrain influence is communicated to the UAM-V through the meteorological inputs. Terrain inputs vary spatially but not temporally, and are generally extracted from the USGS terrain databases, averaging within UAM-V grid cells as necessary. However, since the data is not currently used, AVTERR may be defined as all zeros.

If the LCART flag in the UAM-V control file is set to "true", then this file must also include the latitude/longitude coordinates of the center of each cell of the coarse grid. This binary

(unformatted) data file has a maximum record length of NOX times NOY words. Following the three standard header records, the terrain file follows the record structure below:

Record 1:	((AVTERR(I,J),I=1,NOX),J=1,NOY)	
Record 2:	((CTLON(I,J),I=1,NOX),J=1,NOY)	Include if LCART = .TRUE.
Record 3:	((CTLAT(I,J),I=1,NOX),J=1,NOY)	

AVTERR is the average height of the surface above sea level in meters at each coarse grid cell. CTLON is the longitude of the center of each cell. CTLAT is the latitude of the center of each cell. CTLON and CTLAT determine the location of each cell for use in calculating solar zenith angles.

Meteorological Inputs

Wind Fields (WIND)

The WIND file contains the horizontal wind components (u and v) for each grid cell for each hour of the simulation; these winds determine the transport of simulated pollutants. Additionally, the file defines the surface wind speed at each horizontal grid location (for use in deposition calculations). The vertical (w) wind component is not an input; instead it is calculated directly by the UAM-V from the horizontal wind inputs. Wind fields are usually derived from the output of a meteorological model.

The WIND file is a binary (unformatted) file which has a maximum record length equal to NOX times NOY for the coarse grid or NFX times NFY for a particular fine grid. A WIND file must be supplied for the coarse grid. If it is desired to resolve winds on the fine grids, a separate WIND file must be supplied for each of the fine grids. If no WIND file is supplied for a fine grid, the values for that grid are interpolated from the coarse grid.

The WIND file begins with the three standard header records. Following these records, the record structure for each hour of the WIND coarse-grid file is:

Record 1:	TIME, IDATE	
Record 2:	((U(I,J),I=1,NOX),J=1,NOY)	Repeat NLAYER times
Record 3:	((V(I,J),I=1,NOX),J=1,NOY)	
Record 4:	((WSURF(I,J),I=1,NOX),J=1,NOY)	

U and V are the horizontal wind components in the x- and y-directions respectively in meters per second. WSURF is the surface wind speed in meters per second.

This group of records is repeated as necessary to cover the time span of the simulation at the interval specified in the control file. The record structure is the same for the fine-grid files except that the range on the subscripts is for the size of the fine grid instead of the coarse grid. See the section on the aggregation file for a discussion of how to determine the number of fine-grid cells.

Temperatures (TEMPERATUR)

The TEMPERATUR file defines the absolute temperature (K) for each grid cell for each hour of the simulation. The absolute temperature governs certain chemical reaction rates in the CB-IV chemical mechanism. This file contains the surface temperature and the temperature at the midpoint of each cell in the coarse grid. The temperature may vary spatially and temporally and is usually based on meteorological model output.

The TEMPERATUR file is a binary (unformatted) data file with a maximum record length of 2 plus NOX times NOY. The user provides a TEMPERATUR file for the coarse grid only. Coarse-grid data are interpolated internally by the UAM-V to the fine grids.

The TEMPERATUR file begins with the three standard header records. Following the header records, the record structure of each hour of the TEMPERATUR file is:

Record 1: TIME, IDATE, ((TSURF(I,J),I=1,NOX),J=1,NOY) Record 2: TIME, IDATE, ((TEMPER(I,J),I=1,NOX),J=1,NOY)	Repeat NLAYER times

TSURF is the temperature in kelvins at the surface; TEMPER is the temperature in kelvins at the center of each cell. This group of records is repeated as necessary to cover the time span of the simulation at the interval specified in the control file.

Water Vapor (H2O)

The H2O file contains the concentration of water vapor in parts per million by volume (ppmv) at the midpoint of each cell in the coarse grid. Water vapor concentration may vary spatially and temporally and are usually computed from hourly specific humidity outputs from the meteorological model, vertically averaged within UAM layers, horizontally averaged or interpolated as necessary, and converted to ppmv.

The H2O file is a binary (unformatted) data file with a maximum record length of 2 plus NOX times NOY. The user provides an H2O file for the coarse grid only. Coarse-grid data are interpolated internally by the UAM-V to the fine grids.

The H2O file begins with the three standard header records. Following these records, the record structure of each hour of the H2O file is:

Record 1: TIME, IDATE, ((CH2O(I,J),I=1,NOX),J=1,NOY)	Repeat NLAYER times

CH2O is the average water vapor concentration (ppmv) in each cell. This group of records is repeated as necessary to cover the time span of the simulation at the interval specified in the control file.

Vertical Turbulent Exchange Coefficients (K_v) (VDIFFUSION)

The VDIFFUSION file defines the vertical turbulent exchange coefficients (or diffusivities) in meters squared per second (applicable to all species) at the top of each cell in the grid system for each hour of the simulation. Vertical exchange coefficients may vary spatially and temporally.

The VDIFFUSION file is a binary (unformatted) data file with a maximum record length of 2 plus NOX times NOY. The user must provide a VDIFFUSION file for the coarse grid. The user can optionally provide a separate VDIFFUSION file for any or all of the fine grids. If a VDIFFUSION file is not provided for a fine grid, vertical diffusivities are interpolated internally by the UAM-V to the fine grid from the coarse-grid data.

The VDIFFUSION file begins with the three standard header records. Following these records, the record structure of the coarse-grid VDIFFUSION file is:

Record 1: TIME, IDATE, ((FKV(I,J),I=1,NOX),J=1,NOY)	Repeat NLAYER times

where FKV is the vertical exchange coefficient (m^2/s). The structure of the fine-grid files is the same except that NOX, NOY, and NLAYER are replaced by NFX, NFY, and NFZ respectively. This group of records is repeated as necessary to cover the time span of the simulation at the interval specified in the control file. The vertical exchange coefficients are generated by a prognostic meteorological model or diagnosed from UAM-V wind and temperature inputs (in the WIND and TEMPERATURE files).

Cloud Parameters (CLOUD)

The CLOUD file is an optional file that provides data for two variables: the fractional cloud cover and the cloud liquid water content. If the unit number of the cloud file in the UAM-V control file is zero, the file is not opened or read. A CLOUD file is given for the coarse grid only. Cloud data for fine grids are interpolated from the coarse-grid data. The data may vary spatially and temporally.

This binary (unformatted) data file has a maximum record length of 2 plus NOX times NOY. The CLOUD file begins with the three standard header records. Following these records, the record structure of the file for each hour is:

Record 1: TIME, IDATE, ((CLOUD(I,J),I=1,NOX),J=1,NOY)	Repeat NLAYER times
Record 2: TIME, IDATE, ((CWATER(I,J),I=1,NOX),J=1,NOY)	

This group of records is repeated as necessary to cover the time span of the simulation at the interval specified in the control file.

The CLOUD variable specifies the fractional cloud cover in tenths above each grid cell in the coarse grid. Photolysis rates are adjusted based on this data. The CWATER variable specifies the cloud liquid water content in each cell (g/m^3). This variable may be zero if aqueous phase chemistry calculations are not being performed. The cloud cover may be based on meteorological model output. Alternatively, a preprocessor may be used to interpolate observed sky cover data.

Precipitation Rates (RAIN)

The RAIN file is an optional file that provides data for the rainfall in each horizontal coarse grid cell. If the unit number of the rain file in the UAM-V control file is zero, the file is not opened or read. The data may vary spatially and temporally, but not vertically and is used in calculating wet

deposition rates. A RAIN file is provided for the coarse grid only. Rain data for fine grids are interpolated from the coarse-grid data.

The RAIN file is a binary (unformatted) data file with a maximum record length of 2 plus NOX times NOY. The file begins with the three standard header records. Following these records, the record structure of the file for each hour is:

Record 1: TIME, IDATE, ((RAIN(I,J),I=1,NOX),J=1,NOY)

This record is repeated as necessary to cover the time span of the simulation at the interval specified in the control file. The RAIN variable specifies the rainfall in inches per hour in each layer 1 coarse-grid cell.

Air Quality Inputs

Initial Concentrations (AIRQUALITY)

The AIRQUALITY file contains the initial concentration in parts per million (ppm) of each simulated species in each cell of the coarse grid. Initial concentrations can be developed based on:

- Ambient measurements.
- Previous UAM simulations in the region to be modeled.
- Previous ROM simulations.
- "Clean air" estimates.

Initial condition assumptions often are extremely uncertain. Therefore, it is advisable to ensure enough "start-up" simulation time to remove the influence of the assumed initial conditions on model solutions. The effect of initial-condition uncertainties should be assessed through UAM-V sensitivity experiments.

The AIRQUALITY file is prepared for the coarse grid only. Initial concentrations on fine grids are interpolated from the coarse-grid values. If ROM is exercised for a period that envelops a UAM-V episode, initial conditions for all species may be defined via direct interpolation of ROM concentrations to the UAM-V coarse grid.

The structure of the UAM-V AIRQUALITY file, shown in Table 4-7, is identical to that of the EPA-released version of the UAM (Morris and Myers, 1990). The UAM-IV AIRQUL pre-processor (SAI, 1990) may be used to generate the AIRQUALITY file, but the user must be sure that the layer structure in AIRQUL matches that in the UAM-V.

Lateral Boundary Concentrations (BOUNDARY)

The BOUNDARY file defines the hourly concentration in parts per million of each species for each lateral boundary cell on the coarse grid. The BOUNDARY file also may be used to exclude specified groups of outlying coarse-grid cells from UAM-V calculations.

Lateral boundary concentrations can vary in space and time. If ROM is exercised for a period that envelops a UAM-V episode, boundary conditions for all species may be defined via direct interpolation of ROM concentrations to the UAM-V boundary cells.

Table 4-7.
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 words 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 (**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	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 (the number of segments appears in the File Description Header Record; for the CB-IV version of UAM, 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 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, 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	Concentrations (ppm, or $\mu g/m^3$ for aerosols) for each cell in one vertical level, varying by x-, then y-direction.

The UAM-V BOUNDARY file has the same format as the EPA-released version of the UAM and the BNDARY preprocessor may be used to generate the file. The layers must match the UAM-V layers, however. The record structure is shown in Table 4-8.

Boundary Concentrations at the Top of the Domain (TOPCONC)

The TOPCONC file is an ASCII file that specifies concentrations above the top of the modeling domain for each species. One line is included for each species with each line using the following format:

Species name concentration (ppm) (10A1, F10.7)

Any species that are not included in the file are assigned the lower bound concentration specified in the chemistry parameters file.

Emission Inputs

Point Sources (PTSOURCE)

In the UAM-V a "point" source is an emissions source that is subject to plume rise calculation. An individual source must be designated as a "point" source for its emissions to be injected into UAM-V layers above layer 1.

Table 4-8.
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 words 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 (the 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 (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 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 to be 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 (ppm, or $\mu g/m^3$ for aerosols) 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.

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

- Location.
- Stack parameters (height, diameter, exhaust temperature, flow rate).
- Emissions of each CB-IV species.

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

Note that the UAM-V currently calculates plume rise during simulation, rather than through a preprocessor. After the plume rise calculation, point source emissions that are not treated as plume-in-grid (PiG) are added directly to the relevant grid cell.

The stack diameter parameter in the PTSOURCE file is used as a flag to specify PiG treatment for a source. A source that is treated as PiG with full photochemistry is selected by specifying a negative diameter; any calculations requiring the actual diameter use the absolute value of the diameter. Sources to be treated as PiG with photostationary chemistry are specified by adding 9000 to the diameter and negating the result. A stack with a 10-meter diameter that uses photostationary PiG treatment thus has a specified diameter of -9010.

The PTSRCE preprocessor, Version 1.03 or later, can be used to create the file from the usual ASCII inputs created by the UAM Emissions Preprocessor System (EPS). However, when creating a PTSOURCE file for use with the UAM-V, the vertical method must be STACKHGT rather than PLUMERISE. Input file units in the CONTROL packet should be set to zero.

The format of the PTSOURCE file is identical to the format documented for the EPA-released version of the UAM (Morris and Myers, 1990). The record structure is shown in Table 4-9.

Area Source Emissions (EMISSIONS)

The EMISSIONS file contains total hourly emission rates (into UAM-V layer 1) for each emitted species at each horizontal grid location from a combination of "area" sources, "mobile" sources, and "nonpoint" individual sources. Both anthropogenic and natural source emissions are included in this file.

Three EMISSIONS files can be provided for the coarse grid and each of the fine grids. The first file is used if the current day of the simulation is a weekday, the second file is used if the current day of the simulation is a Saturday, and the third file is used if the day is a Sunday. If the L1EDAY flag is set to true in the UAM-V control file, the date of the EMISSIONS file is not required to match the simulation date. If the unit numbers for the Saturday and Sunday files are zero and the L1EDAY flag is true, the same EMISSIONS file can be used for all days of the simulation.

Table 4-9.
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 words 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.

Fine-grid EMISSIONS files must cover all grid cells of the nested grid system including boundary cells. See the section on the AGGMAP file for a discussion of how to determine the number of fine-grid cells.

Emission files are usually generated with the EPS from the various emissions databases. Biogenic emissions can be generated using the EPA Biogenic Emissions Inventory System (BEIS) or other databases. The EMISSIONS files used by the UAM-V are in a format identical to that used by the EPA release UAM (Morris and Myers, 1990). The record structure is shown in Table 4-10.

Chemistry Input Files

Chemistry Parameters (CHEMPARAM)

The CHEMPARAM file contains information regarding the chemical species to be simulated, including reaction rate constants, upper and lower concentration bounds, and activation energy. The file is supplied with the model and is generally not altered by a user.

The CHEMPARAM file is an ASCII text file whose structure is described in Table 4-11. For photochemical runs, the species to be simulated are required to match a minimum internal set. Only a few gas-phase species are optional for photochemical runs. The species used by the UAM-V and the conditions under which they are required are listed in Table 4-12.

Reaction rates should not be altered from those in the supplied sample file unless the user is intimately familiar with the chemical mechanism. Reaction rates may be omitted for certain inert simulations.

Photolysis Rates (RATES)

The RATES file contains tabulated photolysis rates for seven key reactions: photolysis of NO_2, HCHO (two product channels), O_3 (to form $O(^1D)$), ACET, acrolein, and ALDX. The rates of these reactions vary spatially and temporally; the rates are functions of solar zenith angle, altitude, UV albedo, turbidity, and ozone column density.

A UAM-V preprocessor is used to create a look-up table of photolysis rates spanning all of the conditions that may be encountered during the model run. Photolysis rates are tabulated for 11 altitudes, 10 solar zenith angles, 5 total ozone column values, 5 surface UV albedos and 3 turbidities (i.e., the optical depth due to scattering and absorption of light by aerosols).

The heights above sea level in meters at which the photolysis rates are specified are fixed at 0, 150, 360, 640, 980, 1380, 1840, 2350, 2910, 3530, and 4210. These heights are listed in the data file although the model does not read them. Likewise, the zenith angles for which the photolysis rates are specified are also fixed at 0, 10, 20, 30, 40, 50, 60, 70, 78, 86, and 90 degrees. The values to be used for albedo are set in the file. These values must match the values in the Albedo/Haze/Ozone Column file below. Photolysis rates for the appropriate albedo can then be selected by specifying the corresponding code in the Albedo/Haze/Ozone column file. Similarly, codes are used to select the rates applicable for the local turbidity and ozone column.

The format of the photolysis rates file is described in Table 4-13.

Table 4-10.
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 words 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. Since data in the EMISSIONS file do not vary vertically (all emissions are in the first layer), **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).

Albedo/Haze/Ozone Column (ALBEDO)

The ALBEDO data file is in ASCII format and contains codes for albedo, turbidity, and ozone column density for use in calculating the appropriate photolysis rates. Codes are assigned to five user-specified values of albedo, three values of turbidity, and five values of ozone column density. Albedo codes do not vary temporally and are specified for each coarse-grid cell and optionally for each fine-grid cell; codes for the coarse and all the fine grids are included in the same file.

Data for ozone column and turbidity must be specified on the coarse grid for the entire time span of the simulation. There must be no gaps or overlaps in time spans of each type of data, but spans for turbidity do not need to match those for ozone column. These parameters are not specified for fine grids. Codes for turbidity (or haze) and ozone column density may vary spatially and temporally for the coarse-grid system. Turbidity and ozone column codes for fine grid cells are based on the code for the coarse-grid cell in which the fine-grid cell is located. The format of the Albedo/Haze/Ozone Column file is shown in Table 4-14.

Table 4-11.
Format of UAM-V chemistry parameter file.

Repeat Count	Content	Format	Description
2	Descriptive text	--	Ignored by program.
1	NAM	22X,10A1	File type (must be CHEMPARAM).
1	NID	22X,60A1	File identifier, comment text.
1	NSG	22X,I2	Number of segments (must be 0).
1	NSPEC5	22X,I2	Number of species to be simulated. Must be equal to number of species specified in control file. (See NOSPEC in Tables 3-2 and 3-3)
1	NBDCHP	22X,I2	Ignored by program, may be 0.
1	BTCHP	22X,F2.0	Ignored by program, may be 0.
1	NEDCHP	22X,I2	Ignored by program, may be 0.
1	ETCHP	22X,F2.0	Ignored by program, may be 0.
1	Descriptive text	--	Ignored by program.
NSPEC5	(MSPEC(I,J),I=1,10)	5X,10A1	Species names, one per line.
3	Descriptive text	--	Ignored by program.
1	MMECH	23X,60A1	Mechanism identifier, comment text.
1	LAQ	28X,L4	Aqueous chemistry flag. = .FALSE.
1	LSO2	28X,L4	If = .TRUE., SO2 and sulfate are simulated.
1	LNITR	28X,L4	If = .TRUE., organic nitrate is simulated.
1	LFE	28X,L4	= .FALSE.
1	LMN	28X,L4	= .FALSE.
1	NREACT	37X,I3	Number of gas phase reactions.
1	NAQRAT	37X,I3	Number of aqueous phase reactions. (0)
3	Descriptive text	--	Ignored by program.
NSPEC5	(MSPEC(I,L),I=1,10), LREAC(L), LSSIC(L), LSSBC(L), BDNL(L), BDNU(L)	6X,10A1,3L7,1P 2E17.4	MSPEC = names of species to be simulated. Must match names in prior list.LREAC = reactive species flag; must be .TRUE. for chemically reactive species.LSSIC = Steady State initial conditions flag. .TRUE. only for O3.LSSBC = Steady state boundary conditions flag. .TRUE. only for O3.BDNL = Lower bound for concentrations of this species.BDNU = Upper bound for concentrations of this species (not currently used).
2	Descriptive text	--	Ignored by program.
NREACT	RKN(J), LPHOT(J), LTDEP(J), LPDEP(J), NORDER(J), ACTEN(J), RKN3(J), ACTEN3(J)	5X,1PE12.3,3L6,I 6,3E13.3	RKN = reaction rate in $ppm^{-n}hour^{-1}$.LPHOT = .TRUE. for photolysis reactions.LTDEP = .TRUE. if reaction is temperature dependent.LPDEP = .TRUE. if reaction is pressure dependent.NORDER = order of terms in reaction.ACTEN = activation energy in K.RKN3 = 3rd order reaction rate (for pressure dependent reactions).ACTEN3 = 3rd order reaction activation energy (for pressure dependent reactions).

Table 4-12.
UAM-V internal species names

Species	Part of Minimum Photochemical Set?	Conditions Under Which This Species Is Included
NO	Yes	Photochemical simulation
NO2	Yes	Photochemical simulation
O3	Yes	Photochemical simulation
OLE	Yes	Photochemical simulation
PAR	Yes	Photochemical simulation
TOL	Yes	Photochemical simulation
XYL	Yes	Photochemical simulation
HCHO	Yes	Photochemical simulation
ACET	Yes	Photochemical simulation
ALDX	Yes	Photochemical simulation
CRES	Yes	Photochemical simulation
MGLY	Yes	Photochemical simulation
OPEN	Yes	Photochemical simulation
PNA	Yes	Photochemical simulation
NXOY	Yes	Photochemical simulation
PAN	Yes	Photochemical simulation
PANX	Yes	Photochemical simulation
IOLE	Yes	Photochemical simulation
METH	Yes	Photochemical simulation
CO	Yes	Photochemical simulation
HNO2	Yes	Photochemical simulation
H2O2	Yes	Photochemical simulation
HNO3	Yes	Photochemical simulation
ETOH	No	Photochemical simulation and included in chemistry parameters file
MEOH	No	Photochemical simulation and included in chemistry parameters file
PHCHO	No	Photochemical simulation and included in chemistry paramters file
PACET	No	Photochemical simulation and included in chemistry paramters file
NPHN	No	Photochemical simulation and included in chemistry paramters file
ISOP	No	Photochemical simulation and included in chemistry parameters file (ISPD must also be included.)
ISPD	No	Photochemical simulation and included in chemistry parameters file (ISOP must also be included.)
MTBE	No	Photochemical simulation and included in chemistry parameters file
AER	No	Simulated if included in chemistry parameters file

Table 4-13.
Format for UAM-V photolysis rate file

Repeat enclosed group five times, once for each ozone column class

Repeat enclosed group five times, once for each albedo class

Repeat enclosed group three times, once for each turbidity class

1 line		OZCL, ALBCL, HAZCL: the values of ozone column, albedo, and turbidity used in developing the following photolysis rates	12x,f7.3,8x, f7.3, 11x,f7.3
Repeat 11 times once for each of the 11 heights	1 line	Descriptive text, giving applicable altitude for following rates	A
	7 lines, for NO2, HCHOr, HCHOs, O3-O1D, and ACET, acrolein, and ALDX photolysis	10 values of PRKN on each line, for the angles 0, 10, 20, 30, 40, 50, 60, 70, 78, and 86 degrees (PRKN assumed zero for 90 degrees)	1X,10F12.0

Table 4-14.
Format of UAM-V ALBEDO/HAZE/OZONE COLUMN file.

Repeat Count	Content of line	Format	Description of data
1 line	Descriptive text	A	Text identifying file, creation date, etc.
1 line	MNAME,(ALBCL(I),I= 1,5)	A10, 5F10.0	MNAME must be 'ALBEDO '; the values of ALBCL, the albedo values corresponding to codes 1 through 5, must match those in the photolysis rates file.
1 line	MNAME, (HAZCL(I),I=1,3)	A10, 3F10.0	MNAME must be 'HAZE '; the values of HAZCL, the turbidity values corresponding to codes 1 through 3, must match those in the photolysis rates file.
1 line	MNAME, (OZCL(I),I=1,5)	A10, 5F10.0	MNAME must be 'OZONE COL '; the values of OZCL, the ozone column values corresponding to codes 1 through 5, must match those in the photolysis rates file.
1 line	MNAME, IDD, NXALB, NYALB	A10, 3I10	MNAME must be 'ALBEDO '; IDD is ignored and may be 0; NXALB and NYALB are the number of coarse grid cells in the x- and y-directions and must match NOX and NOY respectively.
NYALB lines	(JALB(I,J),I=1,NXALB)	130I1	Albedo codes, integers in the range 1 to 5. First line is for top (northernmost) row in region (J=NOY) progressing to bottom (southernmost) row (J=1).
1 line	MNAME, IFF, NXALB, NYALB	A10, 3I10	MNAME must be 'ALBEDO '; IFF is fine grid number and if 0, no more albedo codes will be read (a line of this form with IFF = 0 must always be the last line in the albedo section of this file); albedo codes for fine grids must be in numerical order; the number of fine grids for which albedo data is specified may range from 0 to numfin; NXALB and NYALB are the number of fine grid cells in the x- and y-directions for fine grid IFF and must match NFX(IFF) and NFY(IFF) respectively.
NFY(IFF) lines	(JFALB(I,J,IFF),I=1,N FX(IFF))	130I1	Albedo codes, integers in the range 1 to 5. First line is for top (northernmost) row in fine grid IFF (J=NYF(IFF)) progressing to bottom (southernmost) row (J=1).
1 line	MNAME, IDT1, TIM1, IDT2, TIM2	A10, I10,F10.0, I10, F10.0	MNAME must be 'OZONE COL ' or 'HAZE '; IDT1 and TIM1 represent beginning of time span for which data applies; IDT2 and TIM2 represent the end of time span for which data applies. Dates may be calendar dates of the form YYMMDD or Julian dates of the form YYDDD. Times are military times such as 2300. = 11:00 PM.
NOY lines	(JOZC(I,J), I=1,NOX) or (JHAZ(I,J), I=1,NOX)	130I1	Ozone column codes (integers in the range 1 to 5) or turbidity codes (integers in the range 1 to 5) depending on MNAME above. First line is for top (northernmost) row in region (J=NOY) progressing to bottom (southernmost) row (J=1).

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5. MODEL OUTPUT

Text Output

Standard Output File (SYSOUT)

A sample of the data written to standard output during a UAM-V simulation is shown in Exhibit 5-1 starting on page 5-18. (For convenience in referring to exhibits, line numbers are included before the beginning of each line. These line numbers are not normally part of the output.) This file primarily summarizes operational status and timing information for the simulation.

Line 2 of the example notes the version of the model in use. Lines 3 through 31 track initialization of the model including allocation of space for the rolling ozone average. The values of "kind" indicate which of the internal species have been selected for simulation: 0 indicates the internal species is not simulated while any other integer value specifies the number of the internal species in the current simulation. 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.

The warning messages regarding the number of cells in the PTSOURCE file may in general be ignored since the values are not used by the model.

Beginning on line 38, 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. The number of plumes (NPLM) indicates the number of sources treated as Plume-in-Grid (PiG), which in this case is 234. Note that dates on the emission input files are not required to match the modeled dates when the one-day emission input flag is true. (See lines 66–73.)

Steps in the initialization process are noted in lines 176 through 198. 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.

Lines 199 through 202 tally the number of cells that have surface emissions for each of the species in the simulation. Lines 203 through 206 list the number of point sources emitting each species. Line 207 ("Levels:") gives the distribution of point sources according to the vertical layer into which emissions are injected. Note that the number of point sources listed in lines 203–206 may differ from that listed in line 51. 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 lines 213 and 214, in the note for RCHEMF, after the time and date, each group of three numbers represent the maximum, minimum, and average ozone concentration (in ppb) for a level in the fine grid. Line 216 summarizes the steps used in the fine-grid chemistry: time, date, fine-grid advection step in minutes and hours, the maximum, minimum, and average step used in the chemistry solver (in hours), and the maximum, minimum, and average number of

iterations used in the solver. Line 217 prints the K1 RANGE: the maximum, minimum, and average NO2 photolysis rate throughout this fine grid.

In lines 236–248, timing information in CPU seconds for the step just completed for the fine grids is provided. Lines 249–259 provide information similar to that described above for RCHEMF. This information, however, is printed by RCHEM for the coarse grid. Lines 252–256 provide grid cell locations for the maximum and minimum concentrations identified in lines 249–250. Messages on lines 266–291 document puff activity. Finally, lines 295 through 297 summarize CPU time used for the entire time step. ELAPT is the total time used for the step while the number preceding ELAPT is the time used thus far in the simulation. Times are then broken down for subsections of the solution.

Following lines begin to repeat information for the next time step. This information continues to be printed for the duration of the simulation.

Simulation Trace Output (SIMOUT)

The SIMOUT file includes some output that is also included in the standard output file. An example of this file is shown in Exhibit 5-2, starting on page 5-24.

Lines 1 through 6 in the example document the span of the simulation. Lines 7 through 38 document input options and parameters. Following this, some of the diagnostic information included in the standard output is reiterated. This diagnostic information continues during the course of the simulation.

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. An example of a diagnostic file is shown in Exhibit 5-3, starting on page 5-26.

Lines 1 through 69 in the example document the simulation options and some of the data files used. Lines 70 through 229 document the chemistry parameters used in the simulation. The definition of the fine grids and aggregate cells is summarized in lines 230 through 401. More data files and data are documented in lines 403 through 578. In lines 579 through 590, data regarding point sources are tabulated. In the example, the data are tabulated for only the first five sources. However, if the LPRINT flag were set to .TRUE., this information would be included for all sources. Included are the x and y location, the stack height, diameter, temperature, exit velocity, and the PiG flag.

After the information on point sources, emissions totals are included for each grid and each species for both area and point sources (lines 591 through 621). Following these totals, the concentrations at the top of the region, the definition of boundary cells and the initial concentrations are documented (lines 622 through 705). The concentrations at the top of the region are given in parts per million while the initial concentrations are given in micromoles per cubic meter.

Beginning on line 706, 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 (typically at one-hour intervals). It lists boundary concentrations ($\mu mol/m^3$), wind speeds and velocities (km/min), layer height (km), horizontal

diffusion coefficients (km^2/min), vertical exchange coefficients (cm^2/s), and deposition velocities (m/s).

At line 791, the mass flux summary is printed for the fine grids and then for the coarse grid. Since this simulation began at 0000, the mass flux values at 0000 are zeros. Therefore, most of these lines are skipped in the example. Following the mass flux summary, information regarding puffs is tabulated. The tabulation of input values for the following hour and the mass flux summary for 0200 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 portion 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 north, south, east and west boundaries of the grid. Also the flux across the horizontal surface that defines the top boundary of the grid is included. 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. For sources treated as PiG a separate summary is included. "Grid out" records the amount of mass artificially gained after resetting negative grid concentrations resulting from plume dumping to the lower bound value. If this value is not zero or very small, it indicates an operational problem with the PiG treatment, which should be reported to the model developers. The "Plume in" line tells how many moles of NO have been added to grid 1 from plumes that have grown large enough to cease being treated as PiG. "Plume ems" tells the number of moles that have been emitted from sources being treated as PiG. Note that in the coarse grid summary there is an additional line, "Exited", that tells the number of moles advected out of the modeling region in plume form without ever being added to the grid. 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.

Error Message File (ERR)

The error message file includes only warning and error messages including the final error message from the simulation if it did not complete normally. An example of the error message file in Exhibit 5-4 for a case shows an error file with a warning about a point source outside the domain and an error in the date on the wind file, which ended the simulation.

Average Concentrations

Coarse-Grid AVERAGE Concentration File

The coarse grid AVERAGE file is a binary file containing hourly average concentrations (in ppm) of each of the species requested in the control file. The format of the file is the same as the

format of the UAM-IV AVERAGE concentration file (see the "User's Guide to the Urban Airshed Model," 1990). However, the UAM-V 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 (see Table 2-1) in each grid cell for the entire modeling region. The contents of the unformatted AVERAGE file follow the structure for UAM output files and are described in Table 5-1.

Fine-Grid AVERAGE Concentration File

The AVERAGE file is a single binary file containing predicted (typically hourly) average concentrations for all fine grids included in the simulation. The concentrations (ppm) 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 fine-grid AVERAGE file is described in Table 5-2.

Instantaneous Concentrations

Coarse-Grid Instantaneous Concentration File

The coarse-grid INSTANT file includes concentrations for all species in the simulation in micromoles per cubic meter. See the section below on the fine-grid concentration file for a discussion of conversion of concentrations to other units. The full three-dimensional array of coarse-grid cells is included. The format of the file is the same as the format of the UAM-IV AIRQUALITY file (SAI, 1990). The structure of the coarse-grid INSTANT file is given in Table 5-3.

The INSTANT file contains observed concentration values as a function of time for each species over the region (x,y,z).

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 (negative if Lat/lon grid is used)

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 UAM-V**):

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 (ppm, or $\mu g/m^3$ for aerosols) 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) where I specifies the x-cell and J specifies the y-cell.

Table 5-2.
Format of the fine-grid AVERAGE concentration file

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 (ppm) in each cell of layer 1 of the fine grid.

Table 5-3.
Structure of coarse-grid INSTANT file

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 words 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 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	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 ($\mu mol/m^3$ or $\mu g/m^3$ for aerosols) for each cell in one vertical level, varying by x-, then y-direction.

Fine Grid Instantaneous Concentration File

The INSTANTF file contains predicted concentrations for all species in the simulation for all fine grids. This binary file includes concentrations for all layers in micromoles per cubic meter. These concentrations are easily converted to micrograms per cubic meter by multiplying by the appropriate molecular weight. These concentrations can also be converted to parts per million 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,

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

where T is the ambient temperature in degrees K and P is pressure in atmospheres. This conversion can be accomplished using the UAM-V input data files to get the appropriate temperature and pressure, or it can be done approximately assuming T = 298 K and P = 1 atm. In the latter case,

$$(C \text{ in ppm}) = 0.0243\ (C \text{ in } \mu mol/m^3).$$

The structure of the INSTANTF file is described in Table 5-4.

Table 5-4.
Format of the fine grid instantaneous concentration file

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 date either as a calendar date (YYMMDD) or 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 fine 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 (? mol/m^3) in each cell of one layer of the fine grid.

Plume-in-Grid Restart Files

The Plume-in-Grid (PiG) restart files are two binary files each containing information on status of PiG sources and plume segments at one instant in time. If PiG treatment is not being used, the unit numbers for the PiG restart files may be set to zero in the control file and no PiG restart files are written. Otherwise, the user must provide names for two PiG restart files.

PiG restart files can be quite large if a significant number of sources are treated as PiGs. Therefore only 2 hours of PiG information is saved, allowing restart of the UAM-V at each of two hours previous to a planned or unplanned UAM-V termination.

The model will alternately write to one or the other file at the same time as the instantaneous and average concentration files. Before writing to a PiG restart file, it is rewound. One PiG restart file therefore contains the PiG data at the last hour completed in the simulation and the other contains data at the next-to-last hour completed. It is not anticipated that a user would create a PiG restart in any other way than by exercising the UAM-V. However, some of the information on these files may be useful for diagnostic purposes. The format of the files is therefore documented in Table 5-5. The content of variables on the file is documented in Table 5-6.

Sequential Ozone Concentrations

The sequential ozone output file contains the gridded ozone concentrations simulated at each time step of the run. The file is optional and will not be written if the unit number for the file (IUO3) is set to zero in the control file (see Table 4-2). This file is potentially useful for producing animations of the simulated results or calculating average concentrations over periods other than one hour.

The format of this file is described in Table 5-7.

Process Analysis Output Files

Process Analysis (PA) output files are produced if requested by the user. The output files include information on the change in species concentrations due to each of the major processes in the model for the cells selected in the PA control file. Selection of the cells to be included in the output file and the format of the output files are described in detail in the appendix.

Table 5-5.
Format of plume-in-grid restart file

Record No.	Record Length (words)	Variables	Data Types
1	2	TIME, NDATE	Real, Integer
2	12	MXPSPC, MXSKN, MXPFS, MXPLMS, MAXFIN, MXDMP, NPUFFS, NPLM, KCOUNT, NSPEC, NRCLLS, CURTIM	11 Integer followed by 1 Real
3	19*MXPFS	(XLOC(I), YLOC(I), HEIGHT(I), IDUMP(I), DTPUF(I), TPUFF(I), SIGMA(I), SIGMAV(I), KPUFF(I), XLNPUF(I), IFG(I), IIC(I), JJC(I), KKC(I), IIF(I), JJF(I), KKF(I), NPLUME(I), NSRCMBN(I), I=1,MXPFS)	3 Real, Integer, 4 Real, Integer, Real, 9 Integer
4	4*MXPLMS	(XPLM(I), YPLM(I), TSRC(I), NPSRC(I), I=1,MXPLMS)	3 Real, Integer
5	MXPFS*MXPLMS	((ISRCMBN(I,J), I=1,MXPFS), J=1,MXPLMS)	Integer
6	3*MXSKN + 1	(RFACB(I), I=1,MXSKN+1), (RFACC(I), WFAC(I), I=1,MXSKN)	Real
7	MXPSPC*MXPFS	((AML(I,J), I=1,MXPSPC), J=1,MXPFS)	Real
8	MXPSPC*MXPFS	((OAML(I,J), I=1,MXPSPC), J=1,MXPFS)	Real
9	2*MXPFS	(OSGY(I),OSGZ(I), I=1,MXPFS)	Real
10	3*MXPFS	(NSKINS(I), WND(I), TMPRT(I), I=1,MXPFS)	Integer, 2 Real
11	MXPSPC*MXPFS	((EMRATE(I,J), I=1,MXPSPC), J=1,MXPFS)	Real
12	MXPSPC*MXSKN*MXPFS	(((CONCS(I,J,K), I=1,MXPSPC), J=1,MXSKN), K=1,MXPFS)	Real
13	MXPSPC*MXSKN*MXPFS	(((CONNUL(I,J,K), I=1,MXPSPC), J=1,MXSKN), K=1,MXPFS)	Real
14	4*MXDMP* (MAXFIN+1)	((IDMP(I,J), JDMP(I,J), KDMP(I,J), TDMP(I,J), I=1,MXDMP), J=1,MAXFIN+1)	3 Integer, Real
15	MXPSPC*MXDMP	((CONDMP(I,J), I=1,MXPSPC), J=1,MXDMP)	Real
16	2*MXDMP	(VOLDMP(I), DTDMP(I), I=1,MXDMP)	Real
17	MXPSPC*MXPFS	((EPINT(I,J), I=1,MXPSPC), J=1,MXPFS)	Real

Table 5-6.
Definition of variables on the plume-in-grid restart file

Variables	Data Types	Description
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 data that follow applies at this time and date.
MXPSPC, MXSKN, MXPFS, MXPLMS, MAXFIN, MXDMP	Integer	These variables define dimensions of arrays written to file although not all array elements are in use. These variables define number of species, skins, plume segments, plumes (i.e., PiG sources), fine grids, and grid injection locations.
NPUFFS, NPLM	Integer	The actual number of plume segments and plumes in use in the current simulation.
KCOUNT	Integer	The number of plume segments started since the beginning of the simulation.
NSPEC, NRCLLS	Integer	The number of species and number of skins used in the current simulation.
CURTIM	Real	The time in minutes from midnight on the beginning date of the simulation.
XLOC, YLOC	Real	Location of each plume segment (km from coarse grid origin).
HEIGHT	Real	Height of each plume segment above ground (km).
IDUMP	Integer	A flag used internally to identify plume segments to be added to grid system.
DTPUF	Real	The time step (min) at the time when each plume segment was initiated.
TPUFF(I)	Real	If < 0, ABS(TPUFF) is the time at which the plume segment was initiated, measured in minutes from 0000 hours on beginning date of simulation. Otherwise, the interval between the initiation of this plume segment and the initiation of the next plume segment from the same source.
SIGMA, SIGMAV	Real	? $_y$ and ? $_z$, in meters.
KPUFF	Integer	A unique ID number for each plume segment.
XLNPUF	Real	A distance (km) along the direction of travel associated with each plume segment.
IFG	Integer	The number of the most deeply nested fine grid in which each plume segment is located. This value is zero if the plume segment is in the coarse grid only.
IIC, JJC, KKC	Integer	Location of each plume segment in the coarse grid.
IIF, JJF, KKF	Integer	Location of each plume segment in the fine grid identified by IFG.
NPLUME	Integer	Source number from which each plume segment was released.
NSRCMBN	Integer	Number of plume segments from other sources that have been combined into each plume segment.
XPLM, YPLM	Real	Location of each source being treated with PiG wrt the coarse grid origin (km).
TSRC	Real	For each source, the time at which the last plume segment was released.

Variables	Data Types	Description
NPSRC	Integer	Source number of this PiG source in list of all point sources.
ISRCMBN	Integer	For each plume segment, a list of source numbers that have been combined with the segment.
RFACB(I)	Real	For each skin, a factor to multiply σ_y or σ_z by to get distance from plume center to boundary between skin I and I-1.
RFACC(I)	Real	For each skin, a factor to multiply σ_y or σ_z by to get distance from plume center to centerline of skin I.
WFAC(I)	Real	For each skin, factor to multiply σ_y or σ_z by to get width of skin I.
AML(I,J)	Real	Ambient concentrations ($\mu mol/m^3$) of each species used for entrainment by each puff.
OAML(I,J),	Real	Ambient concentrations ($\mu mol/m^3$) of each species used for entrainment by each puff at previous time step.
OSGY, OSGZ	Real	For each plume segment, σ_y and σ_z (m) at previous time step.
NSKINS	Integer	Number of skins currently running for each plume segment.
WND	Real	Wind speed at time of release of each plume segment from source (km/min).
TMPRT	Real	Ambient temperature (K) at the location of each plume segment.
EMRATE	Real	Emissions rate of each species for each plume segment (mol/min).
CONCS(I,J,K)	Real	Concentration ($\mu mol/m^3$) of each species in each skin of each plume segment.
CONNUL(I,J,K)	Real	Concentration ($\mu mol/m^3$) of each species in each skin of each plume segment for zero emissions plume segments.
IDMP(I,J), JDMP(I,J), KDMP(I,J)	Integer	Location in each grid to receive plume mass from plume segments being added to grid system. J=1 corresponds to coarse grid; otherwise, J = fine grid no. + 1.
TDMP(I,J)	Real	For each dumping location, time span (minutes) for which plume mass is to be added to each grid. If 0 or less, this array location is not currently in use.
CONDMP	Real	Rate at which plume mass is to be added to grid system at each dumping location for each species ($\mu mol/min$).
VOLDMP(I)	Real	Volume of plume segment being dumped (km^3).
DTDMP(I)	Real	The step size at initialization for a plume segment being added to grid system.
EPINT	Real	For each plume segment, the total mass of each species loaded into the plume segment at initialization.

Table 5-7.
Structure of the sequential ozone file

Header Records

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

1-10	A	File name = 'O3STEPS '; 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 (= 1).
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 (negative if Lat/lon grid is used)

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 UAM-V**):

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.

(5) The *Fine Grid Number Record* defines the number of nested grids.

1	I	Number of fine grids on file.

(6) The *Fine Grid Description Records* define the location and size of fine grids. One record for each fine grid is included.

1-2	I	x and y beginning coarse grid cell numbers of fine grid.
3-4	I	x and y ending coarse grid cell numbers of fine grid.
5	I	number of fine grid cells per coarse grid cell horizontally.
6	I	number of fine grid cells per coarse grid cell vertically.
7	I	number of cells in x direction in fine grid.
8	I	number of cells in y direction in fine grid.
9	I	number of cells in z direction in fine grid.
10	I	pointer to fine-grid number in which this grid is nested (if 0, then this grid is only within the coarse grid).
11	I	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).

Time-Invariant Data

The O3STEPS file contains no time-invariant data.

Time-Varying Data

The O3STEPS file contains one set of the following records for each time interva1.

(1) The *Steps Record* contains one word for the coarse grid and one word for each fine grid:

1	I	Number of coarse grid steps this period.
2	I	Number of steps for fine grid 1 this period.
(3	I	Number of steps for fine grid 2 this period.)
		(etc.)

The following pair of records is included once for each coarse grid step, then once for each fine grid 1 step, then once for each fine grid 2 step, and so forth.

(2) The *Time Record* contains the time and date at which the concentrations apply:

1	R	Time (hours)
2	I	Date (Julian)

(3) The *Concentration Record* contains the array of ozone concentrations:

1+	R	Concentrations (ppm) at the time specified above for each cell in level one. Values are ordered by x and y location of the cells as follows: ((C(I,J),I=1,NX),J=1,NY) where I specifies the x-cell and J specifies the y-cell. NX and NY are the number of coarse grid cells for coarse grid records, the number of fine grid 1 cells for the fine grid 1 records, and so forth.

Exhibit 5-1.
Example standard output file

```
 1  Mon Mar 20 16:24:02 PST 1995
 2   start model simulation UAM-V v1.23, 12/8/94
 3   open input files
 4  opening control file ir1
 5   initialize model
 6   read surf file        54        48        23
 7   Allocate space for running o3 average.
 8  Allocating     155520 words.  kptr =          1.     1044480 words left.
 9  Allocating     252960 words.  kptr =     155521.      791520 words left.
10  Allocating         60 words.  kptr =     408481.      791460 words left.
11  Allocating         60 words.  kptr =     408541.      791400 words left.
12  Allocating     334800 words.  kptr =     408601.      456600 words left.
13  Allocating         60 words.  kptr =     743401.      456540 words left.
14  Allocating         60 words.  kptr =     743461.      456480 words left.
15  Allocating     123120 words.  kptr =     743521.      333360 words left.
16  Allocating         60 words.  kptr =     866641.      333300 words left.
17  Allocating         60 words.  kptr =     866701.      333240 words left.
18  Allocating      85680 words.  kptr =     866761.      247560 words left.
19  Allocating         60 words.  kptr =     952441.      247500 words left.
20  Allocating         60 words.  kptr =     952501.      247440 words left.
21  Allocating     102000 words.  kptr =     952561.      145440 words left.
22  Allocating         60 words.  kptr =    1054561.      145380 words left.
23  Allocating         60 words.  kptr =    1054621.      145320 words left.
24  Allocating      28080 words.  kptr =    1054681.      117240 words left.
25  Allocating         60 words.  kptr =    1082761.      117180 words left.
26  Allocating         60 words.  kptr =    1082821.      117120 words left.
27  Allocating         60 words.  kptr =    1082881.      117060 words left.
28  Allocating         60 words.  kptr =    1082941.      117000 words left.
29  kind=  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21  0  0  0  0  0  0 22 23  0
30  kind=  0  0  0  0  0  0  0  1
31   read all of input file
32   *** WARNING ***
33   NUMBER OF X CELLS ON PTSOURCE FILE (         108) IS INCORRECT. (          54
34   ).
35   *** WARNING ***
36   NUMBER OF Y CELLS ON PTSOURCE FILE (          96) IS INCORRECT. (          48
37   ).
38   Species   1 NO         on PTSOURCE file = species   1 NO         internally.
39   Species   2 NO2        on PTSOURCE file = species   2 NO2        internally.
40   Species   3 OLE        on PTSOURCE file = species   4 OLE        internally.
```

```
    Species   4 PAR        on PTSOURCE file = species   5 PAR        internally.
    Species   5 TOL        on PTSOURCE file = species   6 TOL        internally.
    Species   6 XYL        on PTSOURCE file = species   7 XYL        internally.
    Species   7 FORM       on PTSOURCE file = species   8 HCHO       internally.
    Species   8 ALD2       on PTSOURCE file = species   9 ALD2       internally.
    Species   9 ETH        on PTSOURCE file = species  10 ETH        internally.
    Species  10 MEOH       on PTSOURCE file = species  22 MEOH       internally.
    Species  11 ETOH       on PTSOURCE file = species  23 ETOH       internally.
    Species  12 ISOP       on PTSOURCE file = species  21 ISOP       internally.
    Species  13 CO         on PTSOURCE file = species  17 CO         internally.
    reading point source data nopts=      7443        36
    finish reading points nplm =       234
    in setup nopts =       7443
    Species   1 NO         on EMISSIONS file = species   1 NO         internally.
    Species   2 NO2        on EMISSIONS file = species   2 NO2        internally.
    Species   3 OLE        on EMISSIONS file = species   4 OLE        internally.
    Species   9 ETH        on EMISSIONS file = species  10 ETH        internally.
  .
  .
  .
  .
    Species  10 MEOH       on EMISSIONS file = species  22 MEOH       internally.
    Species  11 ETOH       on EMISSIONS file = species  23 ETOH       internally.
    Species  12 ISOP       on EMISSIONS file = species  21 ISOP       internally.
    Species  13 CO         on EMISSIONS file = species  17 CO         internally.
    Read interval    88187      0.00 to    88187      1.00 on unit   37
    Read interval    88187      0.00 to    88187      1.00 on unit   80
    Read interval    88187      0.00 to    88187      1.00 on unit   81
    Read interval    88187      0.00 to    88187      1.00 on unit   82
    Read interval    88187      0.00 to    88187      1.00 on unit   84
    Read interval    88187      0.00 to    88187      1.00 on unit   85
    Read interval    88187      0.00 to    88187      1.00 on unit   86
    Read interval    88193      0.00 to    88193      1.00 on unit   36
    call grdsp
    deltax(1), deltay:    47.54668       37.04423
    ifine, delfx(1,ifine), delfy(ifine):
               1   23.14590       18.52211
    ifine, delfx(1,ifine), delfy(ifine):
               2   11.19694       9.261057
    ifine, delfx(1,ifine), delfy(ifine):
               3   10.59610       9.261057
    ifine, delfx(1,ifine), delfy(ifine):
               4   5.424871       4.630528
    ifine, delfx(1,ifine), delfy(ifine):
               5   5.348342       4.630528
```

```
 ifine, delfx(1,ifine), delfy(ifine):
              6   5.270185       4.630528
 File on unit 39 is BOUNDARY
 Species   1 NO         on BOUNDARY   file = species   1 NO         internally.
 Species   2 NO2        on BOUNDARY   file = species   2 NO2        internally.
 Species   3 O3         on BOUNDARY   file = species   3 O3         internally.
 Species   4 OLE        on BOUNDARY   file = species   4 OLE        internally.
 Species   5 PAR        on BOUNDARY   file = species   5 PAR        internally.
 Species   6 TOL        on BOUNDARY   file = species   6 TOL        internally.
 Species   7 XYL        on BOUNDARY   file = species   7 XYL        internally.
 Species   8 HCHO       on BOUNDARY   file = species   8 HCHO       internally.
 Species   9 ALD2       on BOUNDARY   file = species   9 ALD2       internally.
 Species  10 ETH        on BOUNDARY   file = species  10 ETH        internally.
 Species  11 CRES       on BOUNDARY   file = species  11 CRES       internally.
 Species  12 MGLY       on BOUNDARY   file = species  12 MGLY       internally.
 Species  13 OPEN       on BOUNDARY   file = species  13 OPEN       internally.
 Species  14 PNA        on BOUNDARY   file = species  14 PNA        internally.
 Species  15 NXOY       on BOUNDARY   file = species  15 NXOY       internally.
 Species  16 PAN        on BOUNDARY   file = species  16 PAN        internally.
 Species  17 CO         on BOUNDARY   file = species  17 CO         internally.
 Species  18 HONO       on BOUNDARY   file = species  18 HNO2       internally.
 Species  19 H2O2       on BOUNDARY   file = species  19 H2O2       internally.
 Species  20 HNO3       on BOUNDARY   file = species  20 HNO3       internally.
 Species  21 ISOP       on BOUNDARY   file = species  21 ISOP       internally.
 Species  22 MEOH       on BOUNDARY   file = species  22 MEOH       internally.
 Species  23 ETOH       on BOUNDARY   file = species  23 ETOH       internally.
 entering restrt
 opening unit 98 for restart file=/x15/mocauam/uamv/output/conc.moca.run7.880704r            =
 opening unit 99 for fine grid restart file=/x15/mocauam/uamv/output/conc.fgm.moca.run7.880704r=
 fine grid restart file labelled:
  UAMV  run7
 in restrt reading     1700.1     88186
 in restrt reading     1800.1     88186
 in restrt reading     1900.1     88186
 in restrt reading     2000.1     88186
 in restrt reading     2100.1     88186
 in restrt reading     2200.1     88186
 in restrt reading     2300.1     88186
 in restrt reading        0.1    880705
 in restrt     8 outputs skipped         0.     88187
 opening unit 97 for pig restart file=/x15/mocauam/uamv/output/pigout2.run7.880704r           =
 opening unit 97 for pig restart file=/x15/mocauam/uamv/output/pigout2.run7.880704r           =
 pig time:     0.00  880705  search time:     0.00   88187
 time found on pig restart file.
 enter update        0.0    880705(   88187)
```

```
    read mdf         0.0    880705       0.0     88187
    read mdf, fine grid   1         0.0    880705       0.0     88187
    read mdf, fine grid   2         0.0    880705       0.0     88187
    read mdf, fine grid   3         0.0    880705       0.0     88187
    read mdf, fine grid   4         0.0    880705       0.0     88187
    read mdf, fine grid   5         0.0    880705       0.0     88187
    read mdf, fine grid   6         0.0    880705       0.0     88187
    read fzp, fine grid   2         0.0    880705       0.0    880705
    read fzp, fine grid   3         0.0    880705       0.0    880705
    read fzp, fine grid   4         0.0    880705       0.0    880705
    read fzp, fine grid   5         0.0    880705       0.0    880705
    read fzp, fine grid   6         0.0    880705       0.0    880705
    read zp          0.0    880705       0.0     88187
    read fzp, fine grid   2       100.0    880705     100.0    880705
    read fzp, fine grid   3       100.0    880705     100.0    880705
    read fzp, fine grid   4       100.0    880705     100.0    880705
    read fzp, fine grid   5       100.0    880705     100.0    880705
    read fzp, fine grid   6       100.0    880705     100.0    880705
    read zp        100.0    880705       0.0     88187
    read mixht     100.0    880705       0.0     88187
    read temp        0.0    880705       0.0     88187
    Read interval    88187      0.00 to    88187      1.00 on unit   39
    Read HAZE       interval   880701      0.00 to   880712   2400.00 on unit   59
    Read OZONECOL   interval   880701      0.00 to   880701   2400.00 on unit   59
    Read OZONECOL   interval   880702      0.00 to   880702   2400.00 on unit   59
    Read OZONECOL   interval   880703      0.00 to   880703   2400.00 on unit   59
    Read OZONECOL   interval   880704      0.00 to   880704   2400.00 on unit   59
    Read OZONECOL   interval   880705      0.00 to   880705   2400.00 on unit   59
    read fkv, fine grid   1         0.0    880705       0.0    880705
    read fkv, fine grid   2         0.0    880705       0.0    880705
    read fkv, fine grid   3         0.0    880705       0.0    880705
    read fkv, fine grid   4         0.0    880705       0.0    880705
    read fkv, fine grid   5         0.0    880705       0.0    880705
    read fkv, fine grid   6         0.0    880705       0.0    880705
    read kv          0.0    880705       0.0     88187
    read cloud       0.0    880701       0.0     88187
    read cloud     100.0    880701       0.0     88187
   .
   .
    read cloud    2000.0    880704       0.0     88187
    read cloud    2100.0    880704       0.0     88187
    read cloud    2200.0    880704       0.0     88187
    read cloud    2300.0    880704       0.0     88187
    read cloud       0.0    880705       0.0     88187
    read water       0.0    880705       0.0     88187
```

```
 176    TIME STEP SELECTION AT        0.0     88187:      12.00     60.00     25.11    343.07
 177    model initialized cpusecs=      18.1
 178    ENTER AVERAG        0.0     88187     12.00  m =   1
 179    thrs, time =   0.0000000E+00  0.0000000E+00
 180    Placing o3 av concs in location           1
 181    enter avergf        0.0     88187      0.00  m =   1
 182    thrs, time =   0.0000000E+00  0.0000000E+00
 183    Placing o3 av concs in location           1
 184    enter avergf        0.0     88187      0.00  m =   1
 185    thrs, time =   0.0000000E+00  0.0000000E+00
 186    Placing o3 av concs in location           1
 187    enter avergf        0.0     88187      0.00  m =   1
 188    thrs, time =   0.0000000E+00  0.0000000E+00
 189    Placing o3 av concs in location           1
 190    enter avergf        0.0     88187      0.00  m =   1
 191    thrs, time =   0.0000000E+00  0.0000000E+00
 192    Placing o3 av concs in location           1
 193    enter avergf        0.0     88187      0.00  m =   1
 194    thrs, time =   0.0000000E+00  0.0000000E+00
 195    Placing o3 av concs in location           1
 196    enter avergf        0.0     88187      0.00  m =   1
 197    thrs, time =   0.0000000E+00  0.0000000E+00
 198    Placing o3 av concs in location           1
 199     area sources:          2392        2392           0        2392        2392
 200            2392        2392        2392        2392        2392           0
 201               0           0           0           0           0        2392
 202               0           0           0        2392        2392        2392
 203     points:          7097        7097        7097           0        7097        7097
 204            7097        7097        7097        7097        7097           0
 205               0           0           0           0           0        7097
 206               0           0           0        7097        7097        7097
 207     levels:         1899        5138          57           2           1
 208    enter stepx       12.00
 209    enter termsf        0.0     88187     12.00
 210    leave termsf
 211    enter stepxf      12.00
 212    cfrad in rchemf being set for initial values
 213   rchemf      0.00     88187  89   6  45  98  25  54 101  22  57
 214                           93  33  56  78  32  47
 215        tmpinc =   0.0
 216         0.   88187 12.0  0.2000E+00  0.2000E+00  0.2000E+00  0.2000E+00  0.0000E+00  0.0000E+00
       0.0000E+00          13200
 217         0.   88187 k1 range=  0.0000E+00  0.0000E+00  0.0000E+00
 218    enter avergf        0.0     88187     12.00  m =   2
 219    thrs, time =   0.0000000E+00  0.0000000E+00
 220    enter termsf        0.0     88187     12.00
```

```
 leave termsf
 enter stepxf      12.00
rchemf      0.00     88187  77   1  43  78   3  44  92  15  52
                           97   8  56  95  29  55  78  35  49
     tmpinc =   0.0
       0.   88187 12.0  0.2000E+00  0.2000E+00  0.2000E+00  0.2000E+00  0.0000E+00  0.0000E+00
   0.0000E+00          31680
       0.   88187 k1 range=  0.0000E+00  0.0000E+00  0.0000E+00
 enter avergf        0.0     88187     12.00  m =   2
 thrs, time =   0.0000000E+00  0.0000000E+00
 enter termsf        0.0     88187     12.00
 leave termsf
.
.
.
 thrs, time =   0.0000000E+00  0.0000000E+00
  completed fine grids in            2 passes.
 elapsed time for fine grid operations:
   Interpolation:    0.56      diffsf,etc:     0.22
   Transport loop:   63.95 crsfil:    0.94
   stepxf:     8.25  stepyf:    22.85  clvdff:     4.11
   rchemf:   25.94
 total elapsed for each nested grid:
        1       11.11
        2       21.34
        3        7.40
        4        9.77
        5       12.05
        6        3.06
rchem      0.00     88187  83  15  45  91  24  52  93  26  54
                           92  26  51  74  22  43
     tmpinc =   0.0
 at                       14  35       29  39
 at                       23  32       48  11
 at                       38  34       48  11
 at                        6  27       53  19
 at                       40  34       43  30
       0.   88187 12.0  0.2000E+00  0.2000E+00  0.2000E+00  0.2000E+00  0.0000E+00  0.0000E+00
  0.0000E+00          6425
       0.   88187 k1 range=  0.0000E+00  0.0000E+00  0.0000E+00


```

```
 For hour interval  -100.0000     to  0.0000000E+00
 Number of total puff chemistry calls:            0
 Number of times NOx > 10 ppm:            0


 npuff #           20 is dumping            1
 skins because of cross-sectional area
     grid            1  cell           17           7           3
 npuff #           93 is dumping            1
 skins because of cross-sectional area
     grid            0  cell            4          16           3
 npuff #          114 is dumping            1
 skins because of cross-sectional area
     grid            1  cell           18          33           3
 npuff #          115 is dumping            1
 skins because of cross-sectional area
     grid            1  cell           18          33           3
 npuff #          195 is dumping            1
 skins because of cross-sectional area
.
.
.
.
 npuff #         2344 has gotten too big
 npuff #         2369 has gotten too big
 npuff #         2386 has gotten too big
 npuff #         2395 has gotten too big
 npuff #         2449 is dumping            1
 skins because of cross-sectional area
     grid            2  cell            8          79           2
 puff #         195 entering a finer grid
 ENTER AVERAG       12.0     88187     12.00  m =   2
 thrs, time =   0.2000000       12.00000
 Placing o3 av concs in location            2
 TIME STEP SELECTION AT       12.0     88187:      12.00     60.00     25.11    343.07
 End dt    12.0  88187  12.00          111.1 elapt=  92.95
emcors   1.58 hgtnew=   0.13 stepx=   0.99 stepy=   2.66 chem=   1.87
```

Exhibit 5-2
Example SIMOUT file

```
 1  1                    UAMV  run7
 2
 3
 4
 5    Simulation start time/date:           0.      880705
 6    Simulation end time/date:             0.      880706
 7    Data input interval (min):                    100.
 8    Output interval (min):                        100.
 9    Maximum coarse grid time step (min):           15.
10    Minimum hrly avg ozone interval (min):          1.
11
12    Longitude grid spacing:                         1.
13    Latitude grid spacing:                          0.
14    Grid dimensions (x-, y-, z-cells):    54   48    5
15    Number of species:                             23
16
17   wet deposition option =         F
18         restart option  =         T
19   dry deposition option =         T
20            pig option  =         T
21           cart option  =         F
22          inert option  =         F
23     area source option  =         T
24    point source option  =         T
25   one day emiss option  =         T
26   one day inputs option =         F
27   aggregate-cell option =         T
28   dissaggregation method=         2
29   staggered u-v grid op =         F
30   chm time step interval=       1.0
31   Plume-in-Grid parameters:
32      Number of skins:                4
33      Maximum ratio of plume to grid:       0.50
34      Plume combination distance (km):      0.00
35      Puff release interval (min):           30.
36      Puff print interval (min):             60.
37      Maximum puff age (hours):              12.
38   dtmin=   0.000010 maxitr=     5 rerror=   0.020000
39   in restrt     8 outputs skipped       0.     88187
40        0.   88187 12.0  0.2000E+00  0.2000E+00  0.2000E+00  0.2000E+00  0.0000E+00  0.0000E+00
      0.0000E+00          13200
```

```
 41          0.   88187 k1 range=  0.0000E+00  0.0000E+00  0.0000E+00
 42          0.   88187 12.0  0.2000E+00  0.2000E+00  0.2000E+00  0.2000E+00  0.0000E+00  0.0000E+00
         0.0000E+00           31680
 43          0.   88187 k1 range=  0.0000E+00  0.0000E+00  0.0000E+00
 44          0.   88187 12.0  0.2000E+00  0.2000E+00  0.2000E+00  0.2000E+00  0.0000E+00  0.0000E+00
         0.0000E+00           10656
 45          0.   88187 k1 range=  0.0000E+00  0.0000E+00  0.0000E+00
 46          0.   88187  6.0  0.1000E+00  0.1000E+00  0.1000E+00  0.9999E-01  0.0000E+00  0.0000E+00
         0.0000E+00            7680
 47          0.   88187 k1 range=  0.0000E+00  0.0000E+00  0.0000E+00
 48          0.   88187  6.0  0.1000E+00  0.1000E+00  0.1000E+00  0.9999E-01  0.0000E+00  0.0000E+00
         0.0000E+00            9216
 49          0.   88187 k1 range=  0.0000E+00  0.0000E+00  0.0000E+00
 50          0.   88187  6.0  0.1000E+00  0.1000E+00  0.1000E+00  0.1000E+00  0.0000E+00  0.0000E+00
         0.0000E+00            2304
 51          0.   88187 k1 range=  0.0000E+00  0.0000E+00  0.0000E+00
 52          6.   88187  6.0  0.1000E+00  0.1000E+00  0.1000E+00  0.9999E-01  0.0000E+00  0.0000E+00
         0.0000E+00            7680
 53          6.   88187 k1 range=  0.0000E+00  0.0000E+00  0.0000E+00
 54          6.   88187  6.0  0.1000E+00  0.1000E+00  0.1000E+00  0.9999E-01  0.0000E+00  0.0000E+00
         0.0000E+00            9216
 55          6.   88187 k1 range=  0.0000E+00  0.0000E+00  0.0000E+00
 56          6.   88187  6.0  0.1000E+00  0.1000E+00  0.1000E+00  0.1000E+00  0.0000E+00  0.0000E+00
         0.0000E+00            2304
 57          6.   88187 k1 range=  0.0000E+00  0.0000E+00  0.0000E+00
 58     elapsed time for fine grid operations:
 59       Interpolation:    0.56      diffsf,etc:     0.22
 60       Transport loop:   63.95 crsfil:    0.94
 61       stepxf:     8.25  stepyf:    22.85  clvdff:     4.11
 62       rchemf:   25.94
 63     total elapsed for each nested grid:
 64            1       11.11
 65            2       21.34
 66            3        7.40
 67            4        9.77
 68            5       12.05
 69            6        3.06
 70          0.   88187 12.0  0.2000E+00  0.2000E+00  0.2000E+00  0.2000E+00  0.0000E+00  0.0000E+00
          0.0000E+00            6425
 71          0.   88187 k1 range=  0.0000E+00  0.0000E+00  0.0000E+00
 72
 73              time   12.00          totime   12.00          deltat   12.00
 74     End dt    12.0  88187  12.00          111.1 elapt=  92.95
 75    emcors   1.58 hgtnew=   0.13 stepx=   0.99 stepy=   2.66 chem=   1.87
```

```
 ttraj=  17.85 averag=   0.03 update/surlyr=   0.01 Other=   0.00
.
.
.
.
   2354.  880706  6.0  0.1000E+00  0.1000E+00  0.1000E+00  0.1000E+00  0.2000E+01  0.2000E+01
  0.2000E+01           2304
   2354.  880706 k1 range=  0.0000E+00  0.0000E+00  0.0000E+00
 elapsed time for fine grid operations:
   Interpolation:    0.73      diffsf,etc:     0.31
   Transport loop:   83.38 crsfil:    0.94
   stepxf:    10.74  stepyf:    30.22  clvdff:     4.26
   rchemf:   34.34
 total elapsed for each nested grid:
        1       10.69
        2       41.29
        3        7.45
        4        9.89
        5       12.03
        6        3.07
   2348.  880706 12.0  0.2000E+00  0.2000E+00  0.2000E+00  0.2000E+00  0.2000E+01  0.2000E+01
  0.2000E+01           6425
   2348.  880706 k1 range=  0.0000E+00  0.0000E+00  0.0000E+00

         time    0.00          totime 2400.00          deltat   12.00
 End dt     0.0 880706  12.00        16385.9 elapt= 114.26
emcors   0.19 hgtnew=   0.12 stepx=   0.96 stepy=   2.63 chem=   1.91
 ttraj=  18.32 averag=   0.04 update/surlyr=   0.01 Other=   2.58
```

Exhibit 5-3.
Example diagnostic output files

```
 1    open unit=61  file=/x15/mocauam/uamv/output/avrg.moca.run7.880705
       for average conc output
 2    open unit=51= file=/x15/mocauam/uamv/output/conc.moca.run7.880705
       for dump (inst) conc out
 3    open unit=62 file=/x15/mocauam/uamv/output/avrg.fgm.moca.run7.880705
       for fine grid average conc output
 4    open unit=52  file=/x15/mocauam/uamv/output/conc.fgm.moca.run7.880705
       for fine grid inst conc output
 5    open unit=71  file=/x15/mocauam/uamv/output/pigout1.run7.880705
       for pig output restart file
 6    open unit=72  file=/x15/mocauam/uamv/output/pigout2.run7.880705
       for pig output restart file
 7   1                       UAMV  run7
 8
 9
10   PLUME GEOMETRY
11   CELL NO.   1  WIDTH FACTOR-   6.979E-01  CENTERLINE FACTOR-   3.490E-01  BOUNDARY FACTOR-
       0.000E+00
12   CELL NO.   2  WIDTH FACTOR-   3.662E-01  CENTERLINE FACTOR-   8.810E-01  BOUNDARY FACTOR-
       6.979E-01
13   CELL NO.   3  WIDTH FACTOR-   3.819E-01  CENTERLINE FACTOR-   1.255E+00  BOUNDARY FACTOR-
       1.064E+00
14   CELL NO.   4  WIDTH FACTOR-   5.540E-01  CENTERLINE FACTOR-   1.723E+00  BOUNDARY FACTOR-
       1.446E+00
15   INDEX NO.  5                                                             BOUNDARY FACTOR-
       2.000E+00
16
17     Simulation start time/date:            0.      880705
18     Simulation end time/date:              0.      880706
19     Data input interval (min):                     100.
20     Output interval (min):                         100.
21     Maximum coarse grid time step (min):            15.
22     Minimum hrly avg ozone interval (min):           1.
23
24     Longitude grid spacing:                          1.
25     Latitude grid spacing:                           0.
26     Grid dimensions (x-, y-, z-cells):     54   48    5
27     Number of species:                              23
28
29    wet deposition option =          F
30          restart option  =          T
31    dry deposition option =          T
32             pig option  =          T
33            cart option  =          F
34           inert option  =          F
35     area source option  =          T
36    point source option  =          T
37    one day emiss option  =          T
38    one day inputs option =          F
39    aggregate-cell option =          T
40    dissaggregation method=          2
41    staggered u-v grid op =          F
42    chm time step interval=        1.0
43        wlong=  -94.00     elong=  -67.00     slat=   31.00     nlat=   47.00     tzone= 5.0
44        pkrchm=  0.3333E-03          crchem=  0.8333E-04
45
46        chemistry option=         T true=oxidant chemistry, false=linear so2/so4 chemistry
       (nospec=1)
47     advection/diffusion is done using smolarkiewicz
48     long/latitude coordinateosystem
49    horizontal diffusion parameter difcof=             0.2 where kh = difcof * deltay**2 * def
50    maximum and minimum diffusivity =         0.60000        0.00060 km2/min
51    Plume-in-Grid parameters:
52       Number of skins:                4
53       Maximum ratio of plume to grid:        0.50
54       Plume combination distance (km):       0.00
55       Puff release interval (min):            30.
56       Puff print interval (min):              60.
57       Maximum puff age (hours):               12.
58    open unit=10= file=/x15/mocauam/uamv/inputs/rate.moca.in
```

```
        for chem file
 59     open unit=33= file=/x15/mocauam/uamv/inputs/uamv_grdA.wnd.880705.j3
        for mdf file
 60     open unit=34= file=/x15/mocauam/uamv/inputs/uamv_grdA.zp.880705.j3
        for mixht file
 61     open unit=35= file=/x15/mocauam/uamv/inputs/uamv_grdA.tmp.880705.j3
        for temper file
 62     open unit=42= file=/x15/mocauam/uamv/inputs/uamv_grdA.hum.880705.j3
        for water file
 63     open unit=38= file=/x15/mocauam/uamv/inputs/sfc.moca.gridA.new
        for file surf
 64     open unit=36= file=/x15/mocauam/eps2/omef/pts/ptsrce.moca.day.pig.2.bin
        for edf file
 65     open unit=37= file=/x15/mocauam/uamv/inputs/emiss.moca.grdA.880705.a0
        for aem weekday file
 65     open unit=37= file=/x15/mocauam/uamv/inputs/emiss.moca.grdA.880705.a0
        for aem weekday file
 66     open unit=39= file=/dev/null
        for initial conditions
 67     open unit=41= file=/bb4/mocamm/rawdata/ccr_uamV.jul01-11
        for cloud file
 68     open unit=43 file=../inputs/terrain.dummy_b
        for terrain file
 69     open unit=44 file=/x15/mocauam/uamv/inputs/uamv_grdA.kv.880705.j3
        for kv dif file
 70    1***************  CHEMPARAM FILE  ******************
 71    0File description header record
 72         File type      = CHEMPARAM
 73         File id        =   CHEMISTRY PARAMETERS  CBM-IV + AQUEOUS CHEMISTRY
 74         No of segments =  0
 75         No of species  = 23
 76         Beg date       =  0
 77         Beg time       = 0.
 78         End date       =  0
 79         End time       = 0.
 80    0species description header record
 81         NO
 82         NO2
 83         O3
 84         OLE
 85         PAR
 86         TOL
 87         XYL
 88         HCHO
 89         ALD2
 90         ETH
 91         CRES
 92         MGLY
 93         OPEN
 94         PNA
 95         NXOY
 96         PAN
 97         CO
 98         HNO2
 99         H2O2
100         HNO3
101         ISOP
102         MEOH
103         ETOH
104    0chemistry definition record
105         Mechanism id    = CBM-IV  VERSION EPA UAM 6.20 PLUS AQUEOUS
106          lso2=  F lnitr=   F
107         No of gas-phase reactions = 86
108    0species parameters record
109
110         Spec Name   React   SSIC   SSBC            Low Bd Num
111         NO              T      F      F       1.0000E-15
112         NO2             T      F      F       1.0000E-06
113         O3              T      T      T       1.0000E-09
114         OLE             T      F      F       1.0000E-06
115         PAR             T      F      F       1.0000E-04
116         TOL             T      F      F       1.0000E-06
117         XYL             T      F      F       1.0000E-06
118         HCHO            T      F      F       1.0000E-09
119         ALD2            T      F      F       1.0000E-06
120         ETH             T      F      F       1.0000E-06
```

```
121         CRES            T      F      F       1.0000E-06
122         MGLY            T      F      F       1.0000E-06
123         OPEN            T      F      F       1.0000E-12
124         PNA             T      F      F       1.0000E-06
125         NXOY            T      F      F       1.0000E-12
126         PAN             T      F      F       1.0000E-06
127         CO              T      F      F       1.0000E-02
128         HNO2            T      F      F       1.0000E-09
129         H2O2            T      F      F       1.0000E-09
130         HNO3            T      F      F       1.0000E-06
131         ISOP            T      F      F       1.0000E-09
132         MEOH            T      F      F       1.0000E-09
133         ETOH            T      F      F       1.0000E-09
134
135     optional species to be included:
136         Methanol:           T
137         Isoprene:           T
138         Ethanol:            T
139
140      reaction parameters record
141
142           Rate const  Phot  Temp  Pres   #     Act Energy  3rd order  Act Energy
143       1   6.000E+01     T     F     F     1    0.000E+00   0.000E+00    0.000E+00
144       2   2.594E+08     F     T     F     1   -1.175E+03   0.000E+00    0.000E+00
145       3   1.598E+03     F     T     F     1    1.370E+03   0.000E+00    0.000E+00
146       4   8.250E+05     F     F     F     1    0.000E+00   0.000E+00    0.000E+00
147       5   1.385E+05     F     T     F     1   -6.870E+02   0.000E+00    0.000E+00
148       6   1.463E+05     F     T     F     1   -6.020E+02   0.000E+00    0.000E+00
149       7   2.839E+00     F     T     F     1    2.450E+03   0.000E+00    0.000E+00
150       8   5.300E-02     T     F     F     1    0.000E+00   0.000E+00    0.000E+00
151       9   6.000E+01     T     F     F     1    0.000E+00   0.000E+00    0.000E+00
152      10   2.550E+12     F     T     F     1   -3.900E+02   0.000E+00    0.000E+00
153      11   1.956E+07     F     F     F     1    0.000E+00   0.000E+00    0.000E+00
154      12   6.000E+03     F     T     F     1    9.400E+02   0.000E+00    0.000E+00
155      13   1.799E+02     F     T     F     1    5.800E+02   0.000E+00    0.000E+00
156      14   2.034E+03     T     F     F     1    0.000E+00   0.000E+00    0.000E+00
157      15   2.650E+06     F     T     F     1   -2.500E+02   0.000E+00    0.000E+00
158      16   3.541E+01     F     T     F     1    1.230E+03   0.000E+00    0.000E+00
159      17   1.112E+05     F     T     F     1   -2.560E+02   0.000E+00    0.000E+00
160      18   1.140E-04     F     F     F     1    0.000E+00   0.000E+00    0.000E+00
161      19   1.666E+02     F     T     F     1    1.090E+04   0.000E+00    0.000E+00
162      20   9.234E-03     F     T     F     1   -5.300E+02   0.000E+00    0.000E+00
163      21   9.600E-10     F     F     F     1    0.000E+00   0.000E+00    0.000E+00
164      22   5.879E+05     F     T     F     1   -8.060E+02   0.000E+00    0.000E+00
165      23   1.975E-01     T     F     F     1    0.000E+00   0.000E+00    0.000E+00
166      24   5.862E+05     F     F     F     1    0.000E+00   0.000E+00    0.000E+00
167      25   9.000E-04     F     F     F     1    0.000E+00   0.000E+00    0.000E+00
168      26   1.009E+06     F     T     F     1   -7.130E+02   0.000E+00    0.000E+00
169      27   1.307E+04     F     T     F     1   -1.000E+03   0.000E+00    0.000E+00
170      28   7.362E+05     F     T     F     1   -2.400E+02   0.000E+00    0.000E+00
171      29   0.000E+00     F     F     F     1    0.000E+00   0.000E+00    0.000E+00
172      30   0.000E+00     F     F     F     1    0.000E+00   0.000E+00    0.000E+00
173      31   0.000E+00     F     F     F     1    0.000E+00   0.000E+00    0.000E+00
174      32   2.486E+05     F     T     F     1   -1.150E+03   0.000E+00    0.000E+00
175      33   1.309E+01     F     T     F     1   -5.800E+03   0.000E+00    0.000E+00
176      34   2.550E-01     T     F     F     1    0.000E+00   0.000E+00    0.000E+00
177      35   1.512E+05     F     T     F     1    1.870E+02   0.000E+00    0.000E+00
178      36   1.932E+04     F     F     F     1    0.000E+00   0.000E+00    0.000E+00
179      37   9.000E+05     F     F     F     1    0.000E+00   0.000E+00    0.000E+00
180      38   6.000E+01     T     F     F     1    0.000E+00   0.000E+00    0.000E+00
181      39   6.000E+01     T     F     F     1    0.000E+00   0.000E+00    0.000E+00
182      40   1.422E+04     F     T     F     1    1.550E+03   0.000E+00    0.000E+00
183      41   5.580E+01     F     F     F     1    0.000E+00   0.000E+00    0.000E+00
184      42   3.816E+04     F     T     F     1    9.860E+02   0.000E+00    0.000E+00
185      43   1.440E+06     F     T     F     1   -2.500E+02   0.000E+00    0.000E+00
186      44   2.220E+02     F     F     F     1    0.000E+00   0.000E+00    0.000E+00
187      45   6.000E+01     T     F     F     1    0.000E+00   0.000E+00    0.000E+00
188      46   1.692E+06     F     T     F     1    1.800E+02   0.000E+00    0.000E+00
189      47   8.220E+05     F     T     F     1   -3.800E+02   0.000E+00    0.000E+00
190      48   1.524E+00     F     T     F     1    1.350E+04   0.000E+00    0.000E+00
191      49   2.220E+05     F     F     F     1    0.000E+00   0.000E+00    0.000E+00
192      50   5.760E+05     F     F     F     1    0.000E+00   0.000E+00    0.000E+00
193      51   1.260E+03     F     T     F     1    1.710E+03   0.000E+00    0.000E+00
194      52   7.218E+04     F     F     F     1    0.000E+00   0.000E+00    0.000E+00
195      53   8.226E+06     F     T     F     1    8.000E+03   0.000E+00    0.000E+00
196      54   5.727E+06     F     F     F     1    0.000E+00   0.000E+00    0.000E+00
```

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197      55   1.320E+06     F     F     F     1    0.000E+00    0.000E+00    0.000E+00
198      56   3.552E+05     F     T     F     1    3.240E+02    0.000E+00    0.000E+00
199      57   2.520E+06     F     T     F     1   -5.040E+02    0.000E+00    0.000E+00
200      58   1.080E+00     F     T     F     1    2.105E+03    0.000E+00    0.000E+00
201      59   6.810E+02     F     F     F     1    0.000E+00    0.000E+00    0.000E+00
202      60   6.480E+04     F     T     F     1    7.920E+02    0.000E+00    0.000E+00
203      61   7.152E+05     F     T     F     1   -4.110E+02    0.000E+00    0.000E+00
204      62   1.620E-01     F     T     F     1    2.633E+03    0.000E+00    0.000E+00
205      63   5.490E+05     F     T     F     1   -3.220E+02    0.000E+00    0.000E+00
206      64   7.200E+05     F     F     F     1    0.000E+00    0.000E+00    0.000E+00
207      65   1.500E+04     F     F     F     1    0.000E+00    0.000E+00    0.000E+00
208      66   3.660E+06     F     F     F     1    0.000E+00    0.000E+00    0.000E+00
209      67   1.950E+06     F     F     F     1    0.000E+00    0.000E+00    0.000E+00
210      68   1.200E+06     F     F     F     1    0.000E+00    0.000E+00    0.000E+00
211      69   9.040E+00     T     F     F     1    0.000E+00    0.000E+00    0.000E+00
212      70   2.640E+06     F     F     F     1    0.000E+00    0.000E+00    0.000E+00
213      71   9.000E-01     F     T     F     1    5.000E+02    0.000E+00    0.000E+00
214      72   2.172E+06     F     T     F     1   -1.160E+02    0.000E+00    0.000E+00
215      73   1.560E+06     F     F     F     1    0.000E+00    0.000E+00    0.000E+00
216      74   9.640E+00     T     F     F     1    0.000E+00    0.000E+00    0.000E+00
217      75   1.620E+06     F     F     F     1    0.000E+00    0.000E+00    0.000E+00
218      76   8.520E+06     F     F     F     1    0.000E+00    0.000E+00    0.000E+00
219      77   1.080E+00     F     F     F     1    0.000E+00    0.000E+00    0.000E+00
220      78   2.820E+04     F     F     F     1    0.000E+00    0.000E+00    0.000E+00
221      79   7.200E+05     F     F     F     1    0.000E+00    0.000E+00    0.000E+00
222      80   1.200E+05     F     T     F     1   -1.300E+03    0.000E+00    0.000E+00
223      81   6.000E+04     F     F     F     1    0.000E+00    0.000E+00    0.000E+00
224      82   6.660E+04     F     T     F     1   -1.600E+02    0.000E+00    0.000E+00
225      83   4.900E-03     F     F     F     1    0.000E+00    0.000E+00    0.000E+00
226      84   9.600E+04     F     F     F     1    0.000E+00    0.000E+00    0.000E+00
227      85   2.580E+05     F     T     F     1   -1.760E+02    0.000E+00    0.000E+00
228      86   5.340E+05     F     T     F     1   -1.300E+03    0.000E+00    0.000E+00
229     checking chem integration controls...
230     open file=55 file-/x15/mocauam/uamv/inputs/agg.moca.test
         for variable-mesh map
231     entered rvmmap
232        6 fine grids defined.
233     the following definition of fine grids
234     will be used:
235
236
237         horizontal subdivisions:
238
239         00000000000000000000000000000000000000000000000000000000000000
240         00000000000000000000000000000000000000000000000000000000000000
241         00000000000000000000000000000000000000000000000000000000000000
242         00000000000000000000000000000000000000000000000000000000000000
243         00000000000000000000000000000000000000000000000000000000000000
244         00000000000000000000000000000000000000000000000000000000000000
245         00000000000000000000000000000000000000000000000000000000000000
246         00000000000222222222222222222222222222222224444444440000
247         00000000000222222222222222222222222222222224444444440000
248         00000000000222222222222222222222222222222224444444440000
249         00000000000222222222222222244444444444444444444444440000
250         00000000000222222222222222244444444444444444444444440000
251         00000000000222222222222222244444444444444444444444440000
252         00000000000222222222222222244444444444444444444444440000
253         00000000000222222222222222244444444444444444444444440000
254         00000000000222222222222222244444444444444444444444440000
255         00000000000222222222222222244444444444488888844444440000
256         00000000000222222222222222244444444444488888844444440000
257         00000000000222222222222222244444444444488888844444440000
258         00000000000222222222222222244444444444488884444444440000
259         00000000000222222222222222244444444888888880000000000000
260         00000000000222222222222222244444444888888880000000000000
261         00000000000222222222222222244444444888844400000000000000
262         00000000000222222222222222244444444888844400000000000000
263         00000000000222222222222222244444444888844400000000000000
264         00000000000222222222222222244444444444444400000000000000
265         00000000000222222222222222244444444444444400000000000000
266         00000000000222222222222222244444444444444400000000000000
267         00000000000222222222222222244444444444444400000000000000
268         00000000000222222222222222244444444444444400000000000000
269         00000000000222222222222222244444444444444400000000000000
270         00000000000222222222222222244444444444444400000000000000
271         00000000000222222222222222222222222222220000000000000000
```

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272         00000000000022222222222222222222222222220000000000000
273         00000000000022222222222222222222222222220000000000000
274         00000000000022222222222222222222222222220000000000000
275         00000000000022222222222222222222222222220000000000000
276         00000000000022222222222222222222222222220000000000000
277         00000000000022222222222222222222222222220000000000000
278         00000000000022222222222222222222222222220000000000000
279         00000000000000000000000000000000000000000000000000000
280         00000000000000000000000000000000000000000000000000000
281         00000000000000000000000000000000000000000000000000000
282         00000000000000000000000000000000000000000000000000000
283         00000000000000000000000000000000000000000000000000000
284         00000000000000000000000000000000000000000000000000000
285         00000000000000000000000000000000000000000000000000000
286         00000000000000000000000000000000000000000000000000000
287
288         vertical subdivisions:
289
290         00000000000000000000000000000000000000000000000000000
291         00000000000000000000000000000000000000000000000000000
292         00000000000000000000000000000000000000000000000000000
293         00000000000000000000000000000000000000000000000000000
294         00000000000000000000000000000000000000000000000000000
295         00000000000000000000000000000000000000000000000000000
296         00000000000000000000000000000000000000000000000000000
297         00000000000011111111111111111111111111111112222222220000
298         00000000000011111111111111111111111111111112222222220000
299         00000000000011111111111111111111111111111112222222220000
300         00000000000011111111111111122222222222222222222222220000
301         00000000000011111111111111122222222222222222222222220000
302         00000000000011111111111111122222222222222222222222220000
303         00000000000011111111111111122222222222222222222222220000
304         00000000000011111111111111122222222222222222222222220000
305         00000000000011111111111111122222222222222222222222220000
306         00000000000011111111111111122222222222222222222222220000
307         00000000000011111111111111122222222222222222222222220000
308         00000000000011111111111111122222222222222222222222220000
309         00000000000011111111111111122222222222222222222222220000
310         00000000000011111111111111122222222222222220000000000000
311         00000000000011111111111111122222222222222220000000000000
312         00000000000011111111111111122222222222222220000000000000
313         00000000000011111111111111122222222222222220000000000000
314         00000000000011111111111111122222222222222220000000000000
315         00000000000011111111111111122222222222222220000000000000
316         00000000000011111111111111122222222222222220000000000000
317         00000000000011111111111111122222222222222220000000000000
318         00000000000011111111111111122222222222222220000000000000
319         00000000000011111111111111122222222222222220000000000000
320         00000000000011111111111111122222222222222220000000000000
321         00000000000011111111111111122222222222222220000000000000
322         00000000000011111111111111111111111111111110000000000000
323         00000000000011111111111111111111111111111110000000000000
324         00000000000011111111111111111111111111111110000000000000
325         00000000000011111111111111111111111111111110000000000000
326         00000000000011111111111111111111111111111110000000000000
327         00000000000011111111111111111111111111111110000000000000
328         00000000000011111111111111111111111111111110000000000000
329         00000000000011111111111111111111111111111110000000000000
330         00000000000000000000000000000000000000000000000000000
331         00000000000000000000000000000000000000000000000000000
332         00000000000000000000000000000000000000000000000000000
333         00000000000000000000000000000000000000000000000000000
334         00000000000000000000000000000000000000000000000000000
335         00000000000000000000000000000000000000000000000000000
336         00000000000000000000000000000000000000000000000000000
337         00000000000000000000000000000000000000000000000000000
338
339         map of grid id nos.:
340
341         00000000000000000000000000000000000000000000000000000
342         00000000000000000000000000000000000000000000000000000
343         00000000000000000000000000000000000000000000000000000
344         00000000000000000000000000000000000000000000000000000
345         00000000000000000000000000000000000000000000000000000
346         00000000000000000000000000000000000000000000000000000
347         00000000000000000000000000000000000000000000000000000
```

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348         000000000001111111111111111111111111111113333333330000
349         000000000001111111111111111111111111111113333333330000
350         000000000001111111111111111111111111111113333333330000
351         000000000001111111111111112222222222222223333333330000
352         000000000001111111111111112222222222222223333333330000
353         000000000001111111111111112222222222222223333333330000
354         000000000001111111111111112222222222222223333333330000
355         000000000001111111111111112222222222222223333333330000
356         000000000001111111111111112222222222222223333333330000
357         000000000001111111111111112222222222255556633333330000
358         000000000001111111111111112222222222255556633333330000
359         000000000001111111111111112222222222255556633333330000
360         000000000001111111111111112222222222255553333333330000
361         000000000001111111111111112222222444455550000000000000
362         000000000001111111111111112222222444455550000000000000
363         000000000001111111111111112222222444422220000000000000
364         000000000001111111111111112222222444422220000000000000
365         000000000001111111111111112222222444422220000000000000
366         000000000001111111111111112222222222222220000000000000
367         000000000001111111111111112222222222222220000000000000
368         000000000001111111111111112222222222222220000000000000
369         000000000001111111111111112222222222222220000000000000
370         000000000001111111111111112222222222222220000000000000
371         000000000001111111111111112222222222222220000000000000
372         000000000001111111111111112222222222222220000000000000
373         000000000001111111111111111111111111111110000000000000
374         000000000001111111111111111111111111111110000000000000
375         000000000001111111111111111111111111111110000000000000
376         000000000001111111111111111111111111111110000000000000
377         000000000001111111111111111111111111111110000000000000
378         000000000001111111111111111111111111111110000000000000
379         000000000001111111111111111111111111111110000000000000
380         000000000001111111111111111111111111111110000000000000
381         000000000000000000000000000000000000000000000000000000
382         000000000000000000000000000000000000000000000000000000
383         000000000000000000000000000000000000000000000000000000
384         000000000000000000000000000000000000000000000000000000
385         000000000000000000000000000000000000000000000000000000
386         000000000000000000000000000000000000000000000000000000
387         000000000000000000000000000000000000000000000000000000
388         000000000000000000000000000000000000000000000000000000
389    Fine grid          1        62        68         5
390    Fine grid          2        62        90         6
391    Fine grid          3        38        54         6
392    Fine grid          4        34        42         6
393    Fine grid          5        34        50         6
394    Fine grid          6        18        26         6
395    .
396    .
397    .
398    .
399    .
400     from subroutine rvmmap (aggregate cell stuff),
401      11960 aggregate cells verify out of  11960 possible
402
403     open unit 56 file /x15/mocauam/uamv/inputs/uamv_grdB.wnd.880705.j3.extr1
404     for mdf for fine grid  1
405     open unit 53 file /x15/mocauam/uamv/inputs/uamv_grdC.wnd.880705.j1
406     for mdf for fine grid  2
407     open unit 63 file /x15/mocauam/uamv/inputs/uamv_grdD.wnd.880705.j1
408     for mdf for fine grid  3
409     open unit 73 file /x15/mocauam/uamv/inputs/uamv_grdO1.wnd.880705.j1
410     for mdf for fine grid  4
411     open unit 83 file /x15/mocauam/uamv/inputs/uamv_grdO2.wnd.880705.j1
412     for mdf for fine grid  5
413     open unit 93 file /x15/mocauam/uamv/inputs/uamv_grdO3.wnd.880705.j1
414     for mdf for fine grid  6
415     open unit 57 file /x15/mocauam/uamv/inputs/uamv_grdB.kv.880705.j3.extr1
416     for kv for fine grid  1
417     open unit 67 file /x15/mocauam/uamv/inputs/uamv_grdC.kv.880705.j1
418     for kv for fine grid  2
419     open unit 77 file /x15/mocauam/uamv/inputs/uamv_grdD.kv.880705.j1
420     for kv for fine grid  3
421     open unit 87 file /x15/mocauam/uamv/inputs/uamv_grdO1.kv.880705.j1
422     for kv for fine grid  4
423     open unit 91 file /x15/mocauam/uamv/inputs/uamv_grdO2.kv.880705.j1
```

```
 for kv for fine grid  5
 open unit 47 file /x15/mocauam/uamv/inputs/uamv_grdO3.kv.880705.j1
 for kv for fine grid  6
 No file opened for height/pressure for fine grid  1
 open unit 32 file /x15/mocauam/uamv/inputs/uamv_grdC.zp.880705.j1
 for height/pressure for fine grid  2
 open unit 31 file /x15/mocauam/uamv/inputs/uamv_grdD.zp.880705.j1
 for height/pressure for fine grid  3
 open unit 30 file /x15/mocauam/uamv/inputs/uamv_grdO1.zp.880705.j1
 for height/pressure for fine grid  4
 open unit 29 file /x15/mocauam/uamv/inputs/uamv_grdO2.zp.880705.j1
 for height/pressure for fine grid  5
 open unit 28 file /x15/mocauam/uamv/inputs/uamv_grdO3.zp.880705.j1
 for height/pressure for fine grid  6
 open unit 65 file /x15/mocauam/uamv/inputs/sfc.moca.gridB.new
 for surface char. for fine grid  1
 open unit 27 file /x15/mocauam/uamv/inputs/sfc.moca.gridC.new
 for surface char. for fine grid  2
 open unit 26 file /x15/mocauam/uamv/inputs/sfc.moca.gridD.new
 for surface char. for fine grid  3
 open unit 25 file /x15/mocauam/uamv/inputs/sfc.moca.gridO1.new
 for surface char. for fine grid  4
 open unit 24 file /x15/mocauam/uamv/inputs/sfc.moca.gridO2.new
 for surface char. for fine grid  5
 open unit 23 file /x15/mocauam/uamv/inputs/sfc.moca.gridO3.new
 for surface char. for fine grid  6
 open unit 80 file /x15/mocauam/uamv/inputs/emiss.moca.grdB.880705.a0
 for weekday emissions for fine grid  1
 no file opened for saturday emissions for fine grid  1
 no file opened for sunday emissions for fine grid  1
 open unit 81 file /x15/mocauam/uamv/inputs/emiss.moca.grdC.880705.a0
 for weekday emissions for fine grid  2
 no file opened for saturday emissions for fine grid  2
 no file opened for sunday emissions for fine grid  2
 open unit 82 file /x15/mocauam/uamv/inputs/emiss.moca.grdD.880705.a0
 for weekday emissions for fine grid  3
 no file opened for saturday emissions for fine grid  3
 no file opened for sunday emissions for fine grid  3
 open unit 84 file /x15/mocauam/uamv/inputs/emiss.moca.grdO1.880705.a0
 for weekday emissions for fine grid  4
 no file opened for saturday emissions for fine grid  4
 no file opened for sunday emissions for fine grid  4
 open unit 85 file /x15/mocauam/uamv/inputs/emiss.moca.grdO2.880705.a0
 for weekday emissions for fine grid  5
 no file opened for saturday emissions for fine grid  5
 no file opened for sunday emissions for fine grid  5
 open unit 86 file /x15/mocauam/uamv/inputs/emiss.moca.grdO3.880705.a0
 for weekday emissions for fine grid  6
 no file opened for saturday emissions for fine grid  6
 no file opened for sunday emissions for fine grid  6
 Allocate space for running o3 average.
 open unit 59 file /x15/mocauam/uamv/inputs/rates.moca.701-712
 for photolysis rates table.
 read phot values     O3 Column =0.306  Albedo =0.040  Haze O.D. =0.000
 values for height 1   0.000 = Current altitude in km
 values for height 2   0.150 = Current altitude in km
 values for height 3   0.360 = Current altitude in km
 values for height 4   0.640 = Current altitude in km
 values for height 5   0.980 = Current altitude in km
 values for height 6   1.380 = Current altitude in km
 values for height 7   1.840 = Current altitude in km
 values for height 8   2.350 = Current altitude in km
 values for height 9   2.910 = Current altitude in km
 values for height10   3.530 = Current altitude in km
 values for height11   4.210 = Current altitude in km
 read phot values     O3 Column =0.306  Albedo =0.040  Haze O.D. =0.094
 read phot values     O3 Column =0.306  Albedo =0.040  Haze O.D. =0.395
 read phot values     O3 Column =0.306  Albedo =0.050  Haze O.D. =0.000
 read phot values     O3 Column =0.306  Albedo =0.050  Haze O.D. =0.094
 read phot values     O3 Column =0.306  Albedo =0.050  Haze O.D. =0.395
 read phot values     O3 Column =0.306  Albedo =0.060  Haze O.D. =0.000
 read phot values     O3 Column =0.306  Albedo =0.060  Haze O.D. =0.094
 read phot values     O3 Column =0.306  Albedo =0.060  Haze O.D. =0.395
 read phot values     O3 Column =0.306  Albedo =0.070  Haze O.D. =0.000
 read phot values     O3 Column =0.306  Albedo =0.070  Haze O.D. =0.094
 read phot values     O3 Column =0.306  Albedo =0.070  Haze O.D. =0.395
```

```
500     read phot values     O3 Column =0.306  Albedo =0.080  Haze O.D. =0.000
501     read phot values     O3 Column =0.306  Albedo =0.080  Haze O.D. =0.094
502     read phot values     O3 Column =0.306  Albedo =0.080  Haze O.D. =0.395
503     read phot values     O3 Column =0.339  Albedo =0.040  Haze O.D. =0.000
504     read phot values     O3 Column =0.339  Albedo =0.040  Haze O.D. =0.094
505     read phot values     O3 Column =0.339  Albedo =0.040  Haze O.D. =0.395
506     read phot values     O3 Column =0.339  Albedo =0.050  Haze O.D. =0.000
507     read phot values     O3 Column =0.339  Albedo =0.050  Haze O.D. =0.094
508     read phot values     O3 Column =0.339  Albedo =0.050  Haze O.D. =0.395
509     read phot values     O3 Column =0.339  Albedo =0.060  Haze O.D. =0.000
510     read phot values     O3 Column =0.339  Albedo =0.060  Haze O.D. =0.094
511     read phot values     O3 Column =0.339  Albedo =0.060  Haze O.D. =0.395
512     read phot values     O3 Column =0.339  Albedo =0.070  Haze O.D. =0.000
513     read phot values     O3 Column =0.339  Albedo =0.070  Haze O.D. =0.094
514     read phot values     O3 Column =0.339  Albedo =0.070  Haze O.D. =0.395
515     read phot values     O3 Column =0.339  Albedo =0.080  Haze O.D. =0.000
516     read phot values     O3 Column =0.339  Albedo =0.080  Haze O.D. =0.094
517     read phot values     O3 Column =0.339  Albedo =0.080  Haze O.D. =0.395
518     read phot values     O3 Column =0.372  Albedo =0.040  Haze O.D. =0.000
519     read phot values     O3 Column =0.372  Albedo =0.040  Haze O.D. =0.094
520     read phot values     O3 Column =0.372  Albedo =0.040  Haze O.D. =0.395
521     read phot values     O3 Column =0.372  Albedo =0.050  Haze O.D. =0.000
522     read phot values     O3 Column =0.372  Albedo =0.050  Haze O.D. =0.094
523     read phot values     O3 Column =0.372  Albedo =0.050  Haze O.D. =0.395
524     read phot values     O3 Column =0.372  Albedo =0.060  Haze O.D. =0.000
525     read phot values     O3 Column =0.372  Albedo =0.060  Haze O.D. =0.094
526     read phot values     O3 Column =0.372  Albedo =0.060  Haze O.D. =0.395
527     read phot values     O3 Column =0.372  Albedo =0.070  Haze O.D. =0.000
528     read phot values     O3 Column =0.372  Albedo =0.070  Haze O.D. =0.094
529     read phot values     O3 Column =0.372  Albedo =0.070  Haze O.D. =0.395
530     read phot values     O3 Column =0.372  Albedo =0.080  Haze O.D. =0.000
531     read phot values     O3 Column =0.372  Albedo =0.080  Haze O.D. =0.094
532     read phot values     O3 Column =0.372  Albedo =0.080  Haze O.D. =0.395
533     read phot values     O3 Column =0.405  Albedo =0.040  Haze O.D. =0.000
534     read phot values     O3 Column =0.405  Albedo =0.040  Haze O.D. =0.094
535     read phot values     O3 Column =0.405  Albedo =0.040  Haze O.D. =0.395
536     read phot values     O3 Column =0.405  Albedo =0.050  Haze O.D. =0.000
537     read phot values     O3 Column =0.405  Albedo =0.050  Haze O.D. =0.094
538     read phot values     O3 Column =0.405  Albedo =0.050  Haze O.D. =0.395
539     read phot values     O3 Column =0.405  Albedo =0.060  Haze O.D. =0.000
540     read phot values     O3 Column =0.405  Albedo =0.060  Haze O.D. =0.094
541     read phot values     O3 Column =0.405  Albedo =0.060  Haze O.D. =0.395
542     read phot values     O3 Column =0.405  Albedo =0.070  Haze O.D. =0.000
543     read phot values     O3 Column =0.405  Albedo =0.070  Haze O.D. =0.094
544     read phot values     O3 Column =0.405  Albedo =0.070  Haze O.D. =0.395
545     read phot values     O3 Column =0.405  Albedo =0.080  Haze O.D. =0.000
546     read phot values     O3 Column =0.405  Albedo =0.080  Haze O.D. =0.094
547     read phot values     O3 Column =0.405  Albedo =0.080  Haze O.D. =0.395
548     read phot values     O3 Column =0.440  Albedo =0.040  Haze O.D. =0.000
549     read phot values     O3 Column =0.440  Albedo =0.040  Haze O.D. =0.094
550     read phot values     O3 Column =0.440  Albedo =0.040  Haze O.D. =0.395
551     read phot values     O3 Column =0.440  Albedo =0.050  Haze O.D. =0.000
552     read phot values     O3 Column =0.440  Albedo =0.050  Haze O.D. =0.094
553     read phot values     O3 Column =0.440  Albedo =0.050  Haze O.D. =0.395
554     read phot values     O3 Column =0.440  Albedo =0.060  Haze O.D. =0.000
555     read phot values     O3 Column =0.440  Albedo =0.060  Haze O.D. =0.094
556     read phot values     O3 Column =0.440  Albedo =0.060  Haze O.D. =0.395
557     read phot values     O3 Column =0.440  Albedo =0.070  Haze O.D. =0.000
558     read phot values     O3 Column =0.440  Albedo =0.070  Haze O.D. =0.094
559     read phot values     O3 Column =0.440  Albedo =0.070  Haze O.D. =0.395
560     read phot values     O3 Column =0.440  Albedo =0.080  Haze O.D. =0.000
561     read phot values     O3 Column =0.440  Albedo =0.080  Haze O.D. =0.094
562     read phot values     O3 Column =0.440  Albedo =0.080  Haze O.D. =0.395
563     open unit 59 file /x15/mocauam/uamv/inputs/albhzoz.moca.701-712
564     for gridded albedo-haze-ozone column data.
565    ALBEDO-HAZE-OZONE COLUMN      Wed Feb  1 08:10:22 1995
566    ALBEDO         0.0400    0.0500    0.0600    0.0700    0.0800
567    HAZE           0.0000    0.0940    0.3950
568    OZONE COL      0.3060    0.3390    0.3720    0.4050    0.4400
569    ALBEDO         880701        54        48
570    ALBEDO              1        62        68
571    ALBEDO              2        62        90
572    ALBEDO              3        38        54
573    ALBEDO              4        34        42
574    ALBEDO              5        34        50
575    ALBEDO              6        18        26
```

```
 ALBEDO            0         0         0

      7443 point sources are involved in this simulation;  area source emissions=     T
  source number     1
  stack parameters       -91.97     33.14     39.60      2.13    427.00      9.00         F
  source number     2
  stack parameters       -91.97     33.14     42.70      2.44    444.00     12.00         F
  source number     3
  stack parameters       -91.97     33.14     21.30      2.13    450.00     11.00         F
  source number     4
  stack parameters       -91.97     33.14     53.30      3.66    350.00     12.00         F
  source number     5
  stack parameters       -91.96     33.14     73.50      3.96    458.00     18.00         F
  in setup nopts =       7443
  total area and point source emissions (moles/min)
  area    0.9827E+05   0.9356E+04   0.0000E+00   0.7550E+05   0.1327E+07   0.1073E+05
    0.8691E+04   0.3288E+04
    0.7134E+05   0.1068E+05   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00
    0.0000E+00
    0.1009E+07   0.0000E+00   0.0000E+00   0.0000E+00   0.4642E+02   0.2605E+04   0.5211E+04
 point    0.1967E+06   0.2180E+05   0.0000E+00   0.2386E+05   0.9499E+03   0.4031E+03
    0.6524E+03   0.1918E+03
    0.9483E+03   0.3513E+03   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00
    0.0000E+00
    0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   0.1967E+06   0.2180E+05   0.7275E+03
  Emission totals for fine grid     1
  TFAREA= 6.3957E+04 6.3145E+03 0.0000E+00 3.7008E+04 6.9214E+05  7.7023E+03  6.1054E+03
    2.2844E+03              3.2118E+04  7.6666E+03  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  7.1443E+05  0.0000E+00  0.0000E+00
        0.0000E+00  3.2888E+01  1.9602E+03
   3.5952E+03  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
 Emission totals for fine grid     2
  TFAREA= 2.3363E+04 2.3692E+03 0.0000E+00 1.1531E+04 2.1855E+05  2.8441E+03  2.2926E+03
    9.9691E+02  9.9502E+03  3.0179E+03  0.0000E+00
   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  2.8495E+05  0.0000E+00  0.0000E+00
    0.0000E+00  1.2743E+01  3.5386E+02
   6.4660E+02  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
 Emission totals for fine grid     3
  TFAREA= 5.5913E+03 5.8775E+02 0.0000E+00 2.3384E+03 4.7302E+04  7.5674E+02  6.0304E+02
    2.2681E+02  2.3779E+03  4.7046E+02  0.0000E+00
   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  6.8944E+04  0.0000E+00  0.0000E+00
    0.0000E+00  3.3067E+00  7.1126E+01
   1.4586E+02  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
 Emission totals for fine grid     4
  TFAREA= 3.4060E+03 3.6138E+02 0.0000E+00 1.2133E+03 2.4295E+04  3.7989E+02  3.5122E+02
    1.5763E+02  1.1178E+03  3.2730E+02  0.0000E+00
   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  4.4856E+04  0.0000E+00  0.0000E+00
      0.0000E+00  2.2175E+00  5.6018E+01
   7.8948E+01  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
 Emission totals for fine grid     5
  TFAREA= 7.0019E+03 7.5516E+02 0.0000E+00 1.3777E+03 3.7025E+04  7.6950E+02  6.5260E+02
    3.1367E+02  1.2808E+03  6.6344E+02  0.0000E+00
   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  8.4894E+04  0.0000E+00  0.0000E+00
      0.0000E+00  4.0791E+00  7.8730E+01
   2.3645E+02  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
 Emission totals for fine grid     6
  TFAREA= 1.0157E+03 1.0997E+02 0.0000E+00 1.7471E+02 5.5502E+03  1.1560E+02  1.0760E+02
    4.5637E+01  1.9338E+02  8.1161E+01  0.0000E+00
   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  1.4007E+04  0.0000E+00  0.0000E+00
    0.0000E+00  6.4397E-01  7.8225E+00
  open unit=39= file=/x15/mocauam/uamv/inputs/tpc.moca.dat
    for aloft concentrations
  assumed concentrations above top layer=
      NO           0.1000E-05
      NO2          0.1000E-03
      O3           0.4000E-01
      OLE          0.1000E-05
      PAR          0.4000E-02
      TOL          0.6000E-05
      XYL          0.6000E-05
      HCHO         0.1000E-08
      ALD2         0.5000E-04
      ETH          0.1000E-04
      CRES         0.1000E-05
      MGLY         0.1000E-05
```

```
637         OPEN          0.1000E-05
638         PNA           0.1000E-05
639         NXOY          0.1000E-05
640         PAN           0.2000E-03
641         CO            0.1000E+00
642         HNO2          0.1000E-08
643         H2O2          0.1000E-05
644         HNO3          0.1000E-05
645         ISOP          0.1000E-05
646         MEOH          0.1000E-08
647         ETOH          0.1000E-08
648      closed aloft concentration file (unit  39)
649      no file opened for deposition velocities...
650      dry deposition will be calculated internally.
651      open unit=39= file=/x15/mocauam/uamv/inputs/moca.bc.base88.88187.5
          for boundary concentrations
652      boundary definition
653     (***,***)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)
654     (  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)
655     (  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)
656     (  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)
657     (  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(  1, 54)(***,***)(
658     (***,***)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)
659     (  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)
660     (  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)
661     (  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)
662     (  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)(  1, 48)
663     (  1, 48)(  1, 48)(  1, 48)(***,***)(
664      opening unit 98 for restart file=/x15/mocauam/uamv/output/conc.moca.run7.880704r            =
665      opening unit 99 for fine grid restart file=/x15/mocauam/uamv/output/conc.fgm.moca.run7.880704r=
666      fine grid restart file labelled:
667       UAMV  run7
668      opening unit 97 for pig restart file=/x15/mocauam/uamv/output/pigout2.run7.880704r          =
669          at source 2539temps=0.2550E+03This is not a permissible value
670          at source 3032temps=0.2550E+03This is not a permissible value
671          at source 3033temps=0.2550E+03This is not a permissible value
672          at source 3118temps=0.2550E+03This is not a permissible value
673          at source 3876temps=0.2550E+03This is not a permissible value
674          at source 4041temps=0.2550E+03This is not a permissible value
675          at source 4042temps=0.2550E+03This is not a permissible value
676          at source 4930temps=0.2756E+04This is not a permissible value
677          at source 5339temps=0.2033E+04This is not a permissible value
678          at source 5598stkht=0.3000E+00This is not a permissible value
679          at source 5599stkht=0.3000E+00This is not a permissible value
680          at source 5618temps=0.2550E+03This is not a permissible value
681          at source 5620temps=0.2550E+03This is not a permissible value
682          at source 6987temps=0.2550E+03This is not a permissible value
683    1                                  Initial Concentrations
684
685                    Minimum                                          Maximium
        Average
686      layer-  1 NO            0.000000                                    0.022881
         0.000058
687      layer-  2 NO            0.000000                                    0.004874
         0.000002
688      layer-  3 NO            0.000000                                    0.000003
         0.000000
689      layer-  4 NO            0.000000                                    0.000003
         0.000000
690      layer-  5 NO            0.000000                                    0.000002
         0.000000
691      layer-  1 NO2           0.000754                                    1.902638
         0.072798
692      layer-  2 NO2           0.000630                                    0.687639
         0.037663
693      layer-  3 NO2           0.000661                                    0.829975
         0.017378
694      layer-  4 NO2           0.000743                                    0.153460
         0.006271
695      layer-  5 NO2           0.000721                                    0.079813
         0.002331
695      layer-  5 NO2           0.000721                                    0.079813
         0.002331
696      layer-  1 O3            0.676312                                    3.758347
         1.989270
697      layer-  2 O3            1.098651                                    4.098535
```

```
          2.287241
698     layer-  3 O3            1.161846                                4.187288
          2.358000
699     layer-  4 O3            1.159773                                4.142505
          2.231858
700     layer-  5 O3            0.969481                                3.320023
          1.861247
701     .
702     .
703     .
704     .
705     .
706     1     At time    0.   date   88187 updated input variables have the following values
707
708                                    Minimum                                Maximum
          Average
709
710
711     u -layer  1                  -0.23E+00                               0.97E-01
          -0.78E-01
712     v -layer  1                  -0.92E-01                               0.31E+00
          0.10E+00
713     u -layer  2                  -0.39E+00                               0.16E+00
          -0.56E-01
714     v -layer  2                  -0.13E+00                               0.60E+00
          0.17E+00
715     u -layer  3                  -0.48E+00                               0.27E+00
          -0.54E-01
716     v -layer  3                  -0.96E-01                               0.66E+00
          0.17E+00
717     u -layer  4                  -0.51E+00                               0.36E+00
          -0.55E-01
718     v -layer  4                  -0.11E+00                               0.52E+00
          0.11E+00
719     u -layer  5                  -0.37E+00                               0.40E+00
          -0.57E-01
720     v -layer  5                  -0.23E+00                               0.24E+00
          0.18E-01
721     abs(u -layer  1)              0.64E-04                               0.33E+00
          0.25E+00
722     abs(v -layer  1)              0.14E-03                               0.31E+00
          0.11E+00
723     abs(u -layer  2)              0.65E-05                               0.61E+00
          0.33E+00
724     abs(v -layer  2)              0.13E-03                               0.60E+00
          0.17E+00
725     abs(u -layer  3)              0.17E-04                               0.71E+00
          0.36E+00
726     abs(v -layer  3)              0.14E-03                               0.66E+00
          0.18E+00
727     abs(u -layer  4)              0.15E-03                               0.63E+00
          0.36E+00
728     abs(v -layer  4)              0.15E-03                               0.52E+00
          0.12E+00
729     abs(u -layer  5)              0.18E-05                               0.46E+00
          0.35E+00
730     abs(v -layer  5)              0.19E-04                               0.24E+00
          0.73E-01
731     sqr(u( 1)**2+v( 1)**2)        0.82E-02                               0.33E+00
          0.16E+00
732     sqr(u( 2)**2+v( 2)**2)        0.15E-01                               0.61E+00
          0.23E+00
733     sqr(u( 3)**2+v( 3)**2)        0.35E-01                               0.71E+00
          0.24E+00
734     sqr(u( 4)**2+v( 4)**2)        0.52E-02                               0.63E+00
          0.21E+00
735     sqr(u( 5)**2+v( 5)**2)        0.15E-02                               0.46E+00
          0.19E+00
736     wsurf                         0.14E+00                               0.55E+01
          0.27E+01
737     height -layer  1              0.10E+00                               0.10E+00
          0.10E+00
738     height -layer  2              0.50E+00                               0.50E+00
          0.50E+00
739     height -layer  3              0.10E+01                               0.10E+01
          0.10E+01
```

```
740     height -layer  4             0.20E+01                        0.20E+01
          0.20E+01
741     height -layer  5             0.30E+01                        0.30E+01
          0.30E+01
742     kh -layer  1                 0.60E-03                        0.50E+00
            0.13E+00
743     kh -layer  2                 0.60E-03                        0.60E+00
          0.17E+00
744     kh -layer  3                 0.60E-03                        0.56E+00
          0.16E+00
745     kh -layer  4                 0.60E-03                        0.43E+00
          0.12E+00
746     kh -layer  5                 0.60E-03                        0.41E+00
          0.12E+00
747     kv -layer  1                 0.10E+05                        0.30E+05
          0.18E+05
748     kv -layer  2                 0.10E+05                        0.47E+05
          0.11E+05
749     kv -layer  3                 0.10E+05                        0.48E+05
          0.11E+05
750     kv -layer  4                 0.10E+05                        0.23E+05
          0.10E+05
751     kv -layer  5                 0.10E+05                        0.18E+05
          0.10E+05
752     layer  1 temp(k)             0.29E+03                        0.30E+03
          0.30E+03
753     layer  2 temp(k)             0.29E+03                        0.30E+03
          0.30E+03
754     layer  3 temp(k)             0.29E+03                        0.30E+03
          0.29E+03
755     layer  4 temp(k)             0.28E+03                        0.29E+03
          0.29E+03
756     layer  5 temp(k)             0.28E+03                        0.29E+03
          0.28E+03
757     layer  1 h2o(ppm)            0.12E+05                        0.28E+05
          0.19E+05
758     layer  2 h2o(ppm)            0.83E+04                        0.27E+05
           0.16E+05
759     layer  3 h2o(ppm)            0.59E+04                        0.25E+05
          0.15E+05
760     layer  4 h2o(ppm)            0.43E+04                        0.21E+05
          0.13E+05
761     layer  5 h2o(ppm)            0.30E+04                        0.16E+05
          0.87E+04
762     layer  1cloud opacity        0.00E+00                        0.10E+01
          0.14E+00
763     layer  2cloud opacity        0.00E+00                        0.10E+01
          0.14E+00
764     layer  3cloud opacity        0.00E+00                        0.10E+01
          0.14E+00
765     layer  4cloud opacity        0.00E+00                        0.10E+01
          0.14E+00
766     layer  5cloud opacity        0.00E+00                        0.10E+01
          0.14E+00
767     depos. vel. NO                       0.00E+00                        0.00E+00
          0.00E+00
768     layer  1 bc NO         (196 cells)  0.39E-13                        0.93E-06
          0.45E-06
769     layer  2 bc NO         (196 cells)  0.37E-13                        0.10E-05
          0.47E-06
770     layer  3 bc NO         (196 cells)  0.36E-13                        0.95E-06
          0.46E-06
771     layer  4 bc NO         (196 cells)  0.34E-13                        0.12E-05
          0.49E-06
772     layer  5 bc NO         (196 cells)  0.30E-13                        0.12E-05
          0.56E-06
773     depos. vel. NO2                      0.00E+00                        0.00E+00
          0.00E+00
774     layer  1 bc NO2        (196 cells)  0.11E-02                        0.42E+00
          0.41E-01
775     layer  2 bc NO2        (196 cells)  0.10E-02                        0.19E+00
          0.21E-01
776     layer  3 bc NO2        (196 cells)  0.10E-02                        0.51E-01
          0.75E-02
777     layer  4 bc NO2        (196 cells)  0.20E-02                        0.35E-01
          0.61E-02
```

```
778     layer  5 bc NO2        (196 cells)  0.24E-02                          0.24E-01
          0.48E-02
779     depos. vel. O3                      0.00E+00                          0.00E+00
          0.00E+00
780     layer  1 bc O3         (196 cells)  0.12E+01                          0.33E+01
          0.17E+01
781     layer  2 bc O3         (196 cells)  0.13E+01                          0.34E+01
          0.19E+01
782     layer  3 bc O3         (196 cells)  0.13E+01                          0.36E+01
          0.19E+01
783     layer  4 bc O3         (196 cells)  0.12E+01                          0.30E+01
            0.17E+01
784     layer  5 bc O3         (196 cells)  0.11E+01                          0.27E+01
             0.15E+01
785    .
786    .
787    .
788    .
789    .
790
791     Mass flux summary in moles for fine grid  1 at     0.00   88187:
792
793     Spec = NO          North                                          | Spec = NO2         North
794                  In   0.000E+00               Srf emiss  0.000E+00 |              In   0.000E+00
          Srf emiss  0.000E+00
795                  Out  0.000E+00               Elv emiss  0.000E+00 |              Out  0.000E+00
          Elv emiss  0.000E+00
796                  Net  0.000E+00               Depostn    0.000E+00 |              Net  0.000E+00
          Depostn    0.000E+00
797                                                                     |
798            West        Top        East      PIG Mass:              |        West        Top
          East      PIG Mass:
799     In   0.000E+00   0.000E+00   0.000E+00   Grid out   0.000E+00 | In   0.000E+00   0.000E+00
          0.000E+00   Grid out   0.000E+00
800     Out  0.000E+00   0.000E+00   0.000E+00   Plume in   0.000E+00 | Out  0.000E+00   0.000E+00
          0.000E+00   Plume in   0.000E+00
801     Net  0.000E+00   0.000E+00   0.000E+00   Plume ems  0.000E+00 | Net  0.000E+00   0.000E+00
0.000E+00   Plume ems  0.000E+00
802                                                                     |
803                        South                                        |                    South
804                  In   0.000E+00                                     |              In   0.000E+00
805                  Out  0.000E+00               Tot mass   6.124E+03 |              Out  0.000E+00
            Tot mass   9.946E+07
806                  Net  0.000E+00                                     |              Net  0.000E+00
807                                                                     |
808     ------------------------------------------------------------------------------------------------
809     Spec = O3          North                                          | Spec = OLE         North
810                  In   0.000E+00               Srf emiss  0.000E+00 |              In   0.000E+00
          Srf emiss  0.000E+00

811                  Out  0.000E+00               Elv emiss  0.000E+00 |              Out  0.000E+00
          Elv emiss  0.000E+00
812                  Net  0.000E+00               Depostn    0.000E+00 |              Net  0.000E+00
          Depostn    0.000E+00
813                                                                     |

814            West        Top        East      PIG Mass:              |        West        Top
          East      PIG Mass:
815     In   0.000E+00   0.000E+00   0.000E+00   Grid out   0.000E+00 | In   0.000E+00   0.000E+00
          0.000E+00   Grid out   0.000E+00
816     Out  0.000E+00   0.000E+00   0.000E+00   Plume in   0.000E+00 | Out  0.000E+00   0.000E+00
          0.000E+00   Plume in   0.000E+00
817     Net  0.000E+00   0.000E+00   0.000E+00   Plume ems  0.000E+00 | Net  0.000E+00   0.000E+00
          0.000E+00   Plume ems  0.000E+00
818                                                                     |
819                        South                                        |                    South
820                  In   0.000E+00                                     |              In   0.000E+00
840     ------------------------------------------------------------------------------------------------
841    .
842    .
843    .
844    .
845    .
846     ------------------------------------------------------------------------------------------------
847     puff #         108 entering a finer grid
848     puff #         113 entering a finer grid
```

```
 puff #        1373 entering a finer grid
 puff #        1375 entering a finer grid
 puff #        1445 entering a finer grid
 puff #        2344 entering a finer grid

          2381 puffs are currently running.  current time is  1440.00 minutes.
```

pf#	count	sourc	x-y coordinates		height	sigma	sigmav	dmp	releas	delt	t.o.b.	skins
1	2912	27	4.61	16.58	0.99	3223.	192.	0	36.00	12.012	732.00	4
2	2913	32	3.43	16.81	0.92	6983.	259.	0	36.00	12.012	732.00	2
3	2914	84	10.94	12.74	1.03	2815.	184.	0	36.00	12.012	732.00	4
4	2915	149	13.36	9.38	1.15	2549.	179.	0	36.00	12.012	732.00	4
5	2916	211	14.43	8.60	1.33	2858.	185.	0	36.00	12.012	732.00	4
6	2917	214	14.43	8.59	1.33	2857.	185.	0	36.00	12.012	732.00	4
7	2918	236	13.18	9.27	1.09	2434.	176.	0	36.00	12.012	732.00	4
8	5179	27	5.00	15.64	0.74	2018.	163.	0	36.00	12.012	1272.00	4
9	3365	27	4.56	16.20	1.02	2791.	184.	0	36.00	12.012	840.00	4
10	4287	27	4.63	15.49	1.03	2024.	166.	0	36.00	12.012	1056.00	4
11	3980	27	4.58	15.75	1.03	2299.	173.	0	36.00	12.012	984.00	4
12	4135	27	4.60	15.62	1.03	2163.	169.	0	36.00	12.012	1020.00	4

Exhibit 5-4.
Example error output file

271 At source 14xpts=-.3333E+00This is outside the modeling region.

Emissions from this source will not be included in the run.

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Appendix: Description of the Process Analysis Control File and Output Files

Introduction

The UAM[1] and UAM-V models are three-dimensional Eulerian photochemical grid models, designed to simulate the photochemical production of ozone on urban and regional scales. They accomplished this by subdividing the selected modeling domain into fixed grid cells. Within each of these grid cells, and for each chemical species, the species continuity equation is solved by the method of fractional steps. The species continuity equation represents a mass balance in which all of the relevant processes that affect concentrations—emissions, advection, diffusion, chemical reaction, and removal—are included for each species. Each of the individual contributions from these terms (which may be positive or negative) is calculated during the simulation, and the net species concentrations after a time step are retained. Standard UAM and UAM-V output files include gridded fields of the net species concentrations at the top of each hour. The UAM is fully described elsewhere (SAI, 1990).

The Process Analysis (PA) and Integrated Reaction Rate (IRR) extensions to the UAM and UAM-V increase the amount of information that is saved during a photochemical simulation. In addition to the standard UAM or UAM-V output (the net species concentrations), additional information is saved indicating the individual contributions to the net concentrations. Specifically, for each term in the species continuity equation, the changes in concentration due to that term are saved using the PA procedure. This is performed for each species, and each grid cell. Thus, while the standard UAM or UAM-V output allows the user to assess the change in concentration of a species for a particular time and a particular grid cell, the PA technique allows the user to assess the contribution of each process to the concentration change. For instance, while the overall ozone concentration within a grid may not exhibit much change, the PA results may indicate that this is the result of two large terms balancing one another (e.g., vertical transport from aloft versus dry deposition).

For the UAM, the information saved with PA includes: horizontal advection and diffusion across each horizontal cell boundary (4 terms), net horizontal advection and diffusion (1 term), net vertical advection and diffusion across the vertical cell boundaries (1 term), dry deposition onto the surface (1 term), photochemical production or consumption (1 term), chemical titration at night (1 term), surface-level emissions (1 term), elevated point source emissions (1 term), and the final concentration in the cell (1 term).

For the UAM-V, the information saved with PA includes: horizontal advection across each horizontal cell boundary (4 terms), net vertical advection across the vertical cell boundaries (1 term), vertical diffusion across the top of the cell (1 term), vertical diffusion across the bottom of the cell or dry deposition onto the surface (1 term), photochemical production or consumption (1 term), surface-level emissions (1 term), elevated point source emissions

1 UAM is also referred to as UAM-IV.

(1 term), plume-in-grid (P-i-G) injection (1 term), fine-grid to coarse-grid fill-ins (1 term), and the final concentration in the cell (1 term).

The Integrated Reaction Rate (IRR) processor gives information on the mass throughput of each of the reactions in the chemical mechanism, for each hour. After the completion of the photochemical simulation, both the PA and the IRR information are available for display and analysis.

This documentation pertains to versions air6.22.irr of the UAM modeling system, and versions UAMV1.14irr, UAMV1.24irr, and UAM-V 1.30 of the UAM-V modeling system. These three implementations of PA/IRR differ somewhat. Version air6.22.irr is version air6.22 of the UAM with the PA extensions, including the IRR processor. Version UAMV1.14irr uses the standard chemistry solver, and incorporates the IRR processor. Version UAMV1.24irr uses the fast chemistry solver, and does not include the IRR processor. In addition, a post-processing tool, v-post7, is available which allows for extraction of data from the PA/IRR output files. Finally, a graphics package, PAIRRPS, is available separately for graphically displaying the extracted PA and/or IRR information. The implementation and use of each of these software packages is described in the following sections.

System Requirements

The UAM-V version 1.30 model code with PA and IRR capabilities has similar system requirements to those of the more standard versions of the UAM-V. However, the memory overhead is approximately 33 percent greater. The PA extraction code, v-post, has no system requirements beyond those required by the model. The graphics package, PAIRRPS, requires the SAIPLOT libraries. The disk space requirements for the output files can be considerably larger (double or more) than those for standard applications of UAM-V modeling systems.

UAM-V PA/IRR

The UAM-V PA/IRR modeling system is an extension of the UAM-V photochemical modeling system. As such, the facilities and requirements necessary to run the UAM-V PA/IRR modeling system mirror those necessary to run the UAM-V. However, there are additional input requirements, as well as additional output files. These file requirements and formats are described in this section. In all that follows, unless otherwise noted, there are no differences between the implementations for version UAMV1.24irr and version UAMV1.14irr, other than the use of the appropriate executable code.

UAM-V Process Analysis Input Requirements

UAM-V Process Analysis Control File

A sample job stream for running UAMV1.30 was presented above.

UAM-V Process Analysis Input File

The first file indicated in the Control file is the UAM-V PA input file. This file contains all the necessary parameters to specify how the process analysis should be implemented. The format for this file is shown in Table 2-2.

Table A-1.
UAM-V PA input file format

Line #	Content of Line	Data Type	Description of Data
1	comment	a60	comment line
2	lhrout	Logical	if true, then output PA/IRR for the same time blocks as indicated in the UAMV control file (usually hourly); if false, output PA/IRR data for every time step.
3	comment	a60	comment line
4	irr_layer	Int	number of coarse grid vertical layers for PA/IRR data
5... irr_layer+5	irr_ipv(i), i=1,irr_layer	Int	coarse grid layer numbers for PA/IRR data, one layer number per line
irr_layer+6	comment	a60	comment line
irr_layer+7	lcorner	Logical	if true, the desired horizontal coarse grid cells will be indicated by the southwest and northeast corners of a block; if false, the coordinates of each individual cell will be given
IF lcorner is true			
irr_layer+8	ncorner	Int	number of horizontal blocks of coarse grid cells
irr_layer+9	i_sw,j_sw	int,int	x,y cell coordinates of the southwest corner of the first block
irr_layer+10	i_ne,j_ne	int,int	x,y cell coordinates of the northeast corner of the first block
The above two lines are repeated ncorner times.			
IF lcorner is false			
irr_layer+8	irr_grds	int	number of horizontal coarse grid cells for PA/IRR data
irr_layer+9	irr_x(i), irr_y(i)	int,int	x,y cell coordinates of the first cell for PA/IRR output
The above line is repeated irr_grds times			

The vertical layers requested do not have to be contiguous (e.g., one could request layer 1 and layer 5 only), but the layer indices must be valid for a coarse (outer) grid layer. When vertical nesting of fine (inner) grid layers is present, PA/IRR data for all fine grid layers corresponding to a requested coarse grid layer will be saved. Note that in specifying the horizontal cells for PA/IRR data output, 1) all cells are specified with respect to the coarse grid only, and 2) cell coordinates are the cell number, not the latitude/longitude or UTM coordinate. For example, if information for a fine grid cell is desired, and this fine grid cell overlaps coarse grid cell (5,6), then 5,6 are the necessary cell coordinates. If a requested coarse grid cell is overlapped by a fine grid, information for those overlapping fine grid cells will automatically be saved. The fine grid cell's coordinates will be calculated internally, and will be with respect to the origin of that fine grid.

There are two methods for specifying the horizontal grid cells: either as a rectangular block of cells (lcorner = true), or individually (lcorner = false). An example UAM-V PA input file is shown in Table 2-3 for a case where the grid cells are specified by three horizontal boxes. Table 2-4 shows the method used when individually specifying grid cells.

Table A-2.
Example UAM-V PA input file.
This file requests hourly PA/IRR output for three vertical layers, and three horizontal grid boxes.

Control Flag: hourly output (T) or every time step output (F)
T
Vertical layers to be extracted (# of levels, levels)
3
1
2
3
Grid cells: F - specify grid cells, T - sw-ne corners
T
3
27 22
31 26
43 38
47 42
48 43
52 47

Table A-3.
Example UAM-V PA input file
This file requests hourly PA/IRR output for three vertical layers, and five horizontal coarse grid cells.

```
Control Flag: hourly output (T) or every time step output (F)
T
Vertical layers to be extracted (# of levels, levels)
3
1
2
3
Grid cells: F - specify grid cells, T - sw-ne corners
F
5
27 22
27 23
27 24
28 22
28 23
```

The user should be aware that the output files provide approximately 14 times as much output, for each grid cell, as an instantaneous file. Consequently, care should be taken in limiting the number of cells requested to the smallest possible number that will provide the desired information.

UAM-V Process Analysis Output Files

System Output File

There are two files that contain the UAM-V PA and IRR output. In addition to these two files, there is additional run time diagnostic material written to the standard output (SYSOUT) file. This information is related to the proper identification of the grid cells for PA tracking. The user should use this information to confirm, upon model initialization, that the appropriate grid cells have been recognized by the model. Table 2-5 shows an example of the additional UAM-V PA output in a Standard Output file.

Table A-4.
Truncated example of the type of additional output written to the SYSOUT file
This was from a simulation with a 64x63 coarse grid, where 75 coarse grid cells were requested, and each of these coarse grid cells overlapped 9 fine grid cells in the single fine grid. Coarse grid layers 1, 2 and 3 were requested, which overlapped fine grid layers 1 through 5.

```
IPRAM will be printed along with other standard UAM-V outputs
Grid cells: F - specify grid cells, T - sw-ne corners

 Number of dimensions in this simulation is:
   NX =   64
   NY =   63

 Total grid cells in each level =    4032
   # of coarse cells to output =      75
   # of fine   cells to output =     675

 IPRAM coarse grid cell definition:
      1      27      22      0      1
      2      28      22      0      2
      3      29      22      0      3
      4      30      22      0      4
      5      31      22      0      5
      6      27      23      0      6
      7      28      23      0      7
      8      29      23      0      8
      9      30      23      0      9
     10      31      23      0     10
                     ⋮
     71      48      47      0     71
     72      49      47      0     72
     73      50      47      0     73
     74      51      47      0     74
     75      52      47      0     75
```

```
IPRAM fine grid cell definition:
      1      38      11      1      1
      2      39      11      1      2
      3      40      11      1      3
      4      38      12      1      4
      5      39      12      1      5
      6      40      12      1      6
      7      38      13      1      7
      8      39      13      1      8
      9      40      13      1      9
     10      41      11      1     10
     11      42      11      1     11
                     ⋮
    672     115      87      1    672
    673     113      88      1    673
    674     114      88      1    674
    675     115      88      1    675
 vertical layers to be saved:
 grid     layers
   0       1   2   3
   1       1   2   3   4   5
 TIME STEP SELECTION AT       0.0     88187:      12.00      60.00      20.92
343.07
 model initialized cpusecs=      25.5
```

This information is written to the SYSOUT file during model initialization. The lines listing the cell coordinates have data as follows: cell count, x,y,grid id #, internal cell id #. The internal cell id # and the cell count should agree. The user should verify that the horizontal cell coordinates correspond to the expected cell coordinates.

UAM-V Coarse Grid Output File

The PA coarse-grid output file is a binary file which contains the PA and IRR information for each of the coarse grid cells specified in the PA input file, and for each time block over which output was requested. The format of this file is indicated in Table 2-6. Note that since the IRR processor is not implemented in version UAMV1.24irr, the IRR values have all been set to zero for this version.

Table A-5.
Format of the coarse grid PA/IRR output file

Record #	Variables	Data Type	Description	
Time Invariant Information – written once				
1	nx,ny,nz	int,int,int	x,y,z dimensions of the coarse grid	
2	nests,(ilyr(i),i =1,nests), igc,igf	All integer	nests -	the number of fine grids with PA/IRR information
			ilyr(i) -	the number of vertical layers, for fine grid i, with PA/IRR data. Note i is just a sequential counter, not the UAM-V grid index number.
			igc -	total number of coarse grid cells per horizontal layer with PA/IRR information
			igf -	total number of fine grid cells per horizontal layer with PA/IRR information
Time Varying Information – written for each time block				
3	noxy,mz, nspec,irrsp, nreact,ttime, ldark	int,int, int,int, int,real, logical	noxy -	total number of coarse grid cells per horizontal layer
			mz -	total number of vertical layers for the coarse grid
			nspec -	total number of chemical species
			irrsp -	number of species for which PA/IRR information is reported (=nspec)
			nreact -	total number of chemical reactions
			ttime -	time for this data block
			ldark -	true=night, false=day
4	((mspec(i,j), i=1,10), j=1,irrsp)	integer (or character*4)	list of species names, each name 10 characters long, with one character per word	
Repeat all that follows igc times				
5	nlayers	Int	then number of vertical layers with PA/IRR data for the following cell	

Record #	Variables	Data Type	Description	
Repeat all that follows nlayers times				
6	ipv,iphx, iphy,ipcf	All integer	ipv -	vertical UAM-V layer of this coarse grid cell
			iphx -	x coordinate of this coarse grid cell
			iphy -	y coordinate of this coarse grid cell
			ipcf -	UAM-V grid identifier (=0 for coarse grid)
7	rate_irr(i), i=1,nreact	Real	IRR information for this cell, for reactions 1,...,nreact	
8	chem(i), wflux(i), eflux(i), sflux(i), nflux(i), bottom(i), tdiff(i), lemis(i), pemis(i), pig(i), clorz(i), fillin(i), final(i), i=1,irrsp	All real	chem(i) -	chemistry PA information for this grid cell for species i
			wflux(i) -	western cell boundary advection for this grid cell
			eflux(i) -	eastern cell boundary advection for this grid cell
			sflux(i) -	southern cell boundary advection for this grid cell
			nflux(i) -	northern cell boundary advection for this grid cell
			bottom(i) -	for vertical layer 1, dry deposition for this cell; for other layers, vertical diffusion across the bottom of the cell
			tdiff(i) -	vertical diffusion across the top of this grid cell
			lemis(i) -	low level emission in this grid cell
			pemis(i) -	elevated emission in this grid cell
			pig(i) -	Plume-in-Grid injection in this grid cell
			clorz(i) -	net vertical advection across the top and bottom of this grid cell
			fillin(i) -	fine-grid to coarse-grid fill-in for this grid cell
			final(i) -	final PA species concentrations i in this grid cell

UAM-V Fine Grid Output File

The PA fine-grid output file is a binary file that contains the PA and IRR information for each fine-grid cell that is contained within a coarse-grid cell indicated in the PA input file. The structure of this file is similar to that of the coarse-grid output file, and is indicated in Table 2-7.

Table A-6.
Format of the fine grid PA/IRR output file

Record #	Variables	Data Type	Description	
Time Invariant Information - written once				
1	nx,ny,nz	int,int,int	x,y,z dimensions of the coarse grid	
2	nests,(ilyr(i),i =1,nests), igc,igf	All integer	nests -	the number of fine grids with PA/IRR information
			ilyr(i) -	the number of vertical layers, for fine grid i, with PA/IRR information. Note i is just a sequential counter, not the UAM-V grid index number.
			igc -	total number of coarse grid cells per horizontal layer with PA/IRR information
			igf -	total number of fine grid cells per horizontal layer with PA/IRR information
Time Varying Information - written for each time block				
3	noxy,mz, nspec,irrsp, nreact,ttime, ldark	int,int, int,int, int,real, logical	noxy -	total number of coarse grid cells per horizontal layer
			mz -	total number of vertical layers for the coarse grid
			nspec -	total number of chemical species
			irrsp -	number of species for which PA/IRR information is reported (=nspec)
			nreact -	total number of chemical reactions
			ttime -	time for this data block
			ldark -	true=night, false=day
4	((mspec(i,j), i=1,10), j=1,irrsp)	character*10	list of species names, each name 10 characters long, with one character per word	
Repeat all that follows igf times				
5	nlayers	Int	then number of vertical layers with PA/IRR information for the following cell	
Repeat all that follows nlayers times				

Record #	Variables	Data Type	Description	
6	ipv,iphx, iphy,ipcf	All integer	ipv -	vertical UAM-V layer of this fine grid cell
			iphx -	x coordinate of this fine grid cell
			iphy -	y coordinate of this fine grid cell
			ipcf -	UAM-V grid identifier (≥1 for fine grid)
7	rate_irr(i), i=1,nreact	All real	IRR information for this cell, for reactions 1,...,nreact	
8	chem(i), wflux(i), eflux(i), sflux(i), nflux(i), bottom(i), tdiff(i), lemis(i), pemis(i), pig(i), clorz(i), fillin(i), final(i), i=1,irrsp	All real	chem(i) -	chemistry PA information for this grid cell for species i
			wflux(i) -	western cell boundary advection for this grid cell
			eflux(i) -	eastern cell boundary advection for this grid cell
			sflux(i) -	southern cell boundary advection for this grid cell
			nflux(i) -	northern cell boundary advection for this grid cell
			bottom(i) -	for vertical layer 1, dry deposition for this cell; for other layers, vertical diffusion across the bottom of the cell
			tdiff(i) -	vertical diffusion across the top of this grid cell
			lemis(i) -	low level emissions in this grid cell
			pemis(i) -	elevated emissions in this grid cell
			pig(i) -	Plume-in-Grid injection in this grid cell
			clorz(i) -	net vertical advection across the top and bottom of this grid cell
			fillin(i) -	fine-grid to coarse-grid fill-in for this grid cell
			final(i) -	final PA species concentrations i in this grid cell

These two output files allow for a wide range of process-related analyses subsequent to simulation completion.

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