

**USER'S GUIDE TO THE
COMPREHENSIVE AIR QUALITY MODEL
WITH EXTENSIONS (CAM_x)**

Version 1.10

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1. OVERVIEW OF CAMx

CAMx is a new three-dimensional Eulerian photochemical grid model designed to calculate the spatial and temporal concentration distribution of both inert and chemically reactive gaseous pollutants by simulating processes associated with emissions, transport, chemistry, and removal. CAMx is based on the atmospheric continuity equation, which represents a balance between local pollutant concentrations and all of the relevant physical and chemical processes impacting that point. This equation can be expressed mathematically in terrain-following height (z) coordinates as:

$$\begin{aligned} \frac{\partial c_l}{\partial t} = & -(\nabla_H \cdot \vec{V}_H c_l) + \left[\frac{\partial(c_l \eta)}{\partial z} - c_l \frac{\partial(\eta + w)}{\partial z} \right] + (\nabla \cdot K \nabla c_l) \\ & + \left. \frac{\partial c_l}{\partial t} \right|_{Chemistry} + \left. \frac{\partial c_l}{\partial t} \right|_{Emission} + \left. \frac{\partial c_l}{\partial t} \right|_{Removal} \end{aligned}$$

where c_l is the three-dimensional concentration of pollutant species l at time t , V_H is the horizontal wind vector, w is the vertical velocity, and K is the turbulent diffusion coefficient (given separately for horizontal and vertical coordinates). The first term on the right-hand side represents horizontal advection, while the second term represents vertical transport. As the vertical grid structure is defined via external inputs, layer heights may be specified as a any arbitrary function of time and/or space. Total vertical transport is therefore the net effect of vertical advection, mass exchange between layers due to entrainment, and concentration change due to dilution. The local entrainment rate η is a combination of vertical velocity and the total (Lagrangian) time rate of change of the layer interface heights h :

$$\eta = \frac{\partial h}{\partial t} + (\vec{V}_H \cdot \nabla_H h) - w$$

The continuity equation is solved using the method of fractional steps (or time-splitting) in which each major process (advection, diffusion, chemistry) is solved in independent sequence. The model is integrated forward in time using a driving time step that ensures numerical stability of the coarse grid horizontal advection and diffusion. Therefore, the maximum time step is a function of the coarse grid size, wind speed, and horizontal diffusion coefficient. Typical time steps for grid spacing of 10-50 km are 10-30 minutes, whereas time steps for grid spacing of 1-2 km are several minutes or less. Therefore, multiple advective time steps per driving step are required for the finer nested grids depending on their size relative to coarse grid spacing. Multiple chemistry time steps per driving step are usually needed as well to ensure stable solutions of the often very stiff chemical reaction equations.

In addition to the features it shares with most photochemical grid models, the most notable new features of CAMx are:

- **Nested Grid Structure:** This feature allows CAMx to be run with coarse grid spacing over a wide regional domain in which high spatial resolution is not particularly needed, while within the same run, applying fine grid nests in areas where they are needed;

- Fast Plume-in-Grid (PiG) Module: CAMx incorporates a PiG feature to adequately model the chemistry of point source NO_x plumes; individual plume segments are tracked while undergoing dispersion and chemical evolution, until such time as they can be adequately represented within the grid model framework;
- Fast Numerical Chemical Kinetics Solver: ENVIRON has developed a highly efficient chemistry solver that is based on an “adaptive-hybrid” approach; relative to the standard chemistry solvers, the approach results in about a ten-fold speedup in the chemistry solution and an overall model speedup by a factor of 3 to 4;
- Source Apportionment: Allows CAMx to track source region or source category contributions to predicted grid cell ozone concentration; thus, for any selected receptor point and time, the model gives a clear picture of the likely distribution of ozone and ozone precursors by source category and/or source region, as well as an indication as to whether the ozone at the selected time and location would more likely respond to upwind NO_x or VOC controls.

2. DESCRIPTION OF CAMx FORMULATION

The following sections describe the technical formulation of the major CAMx components. CAMx v1.10 software includes new coding of several industry-accepted algorithms and component formulations, while its modular framework permits easy substitution of new and/or improved algorithms in the future.

POLLUTANT TRANSPORT

Horizontal advection is performed using the forward-upstream diffusive-corrected algorithm of Smolarkiewicz (1983). Several other algorithms have exhibited less numerical diffusion than the Smolarkiewicz algorithm, however, at an increased computation time (Chock, 1991). When used in other modeling platforms, some of these other advection algorithms have produced significant differences in ozone predictions from those generated using the Smolarkiewicz algorithm. Later versions of CAMx will incorporate optional advection schemes. Vertical transport is accomplished through the use of a multi-cycle Lorentz scheme, which adjusts the column concentration profile of a given species via resolved vertical velocity (as determined from the divergence of the horizontal winds), and the time- and space-variations of the vertical grid structure (as defined by the input layer heights).

Explicit horizontal diffusion is calculated through a simple flux-divergence calculation added at the end of the Smolarkiewicz advection code; i.e., horizontal diffusion along the length of a particular row or column is applied after advective integration. Horizontal diffusion coefficients are determined internally using the deformation approach of Smagorinsky (1963). Vertical diffusion is calculated using an implicit numerical approach, which requires the inversion of a tri-diagonal matrix. As this approach is absolutely numerically stable, only one diffusion step is required per driving time step. Explicit approaches require potentially many more diffusion steps (on the order of 10-100) to maintain a stable solution. Gridded vertical diffusion coefficients are supplied to the model via an hourly input file.

CAMx incorporates two-way nested grid capabilities. Two-way nesting means that pollutant concentration information propagates into and out of all fine grid nests. Any number of grid nests can be specified in a single run, while grid spacings and vertical layer structures can vary from one grid nest to another. The nested grid capability of CAMx allows it to be cost-effectively applied to large regions in which regional transport occurs, yet at the same time provide fine resolution sufficient to address small-scale impacts.

The current restrictions on specifying the size and resolution of all grid nests include the following:

- 1) The ratio of coarse grid cell size to fine grid cell size must be an integer (e.g., a “meshing factor” of 3 means that 3 fine grid cells span the distance of 1 coarse grid cell, resulting in an area of 9 fine grid cells per coarse grid cell);
- 2) Fine grids cannot overlap, although they may share a common boundary or edge;
- 3) Fine grids cannot extend into a boundary, or non-modeled, area of the coarse grid;

- 4) CAMx is currently configured to allow four “generations” of nests (e.g., four levels of telescoping grids); this can be extended in the code easily if more than four levels of nests are required;
- 5) The vertical depth (i.e., region top) of each fine grid must exactly match the depth of the coarse grid;
- 6) Fine grid vertical layers may exactly match the coarse grid vertical structure, or the coarse grid layers may be individually split into several fine grid layers (defined via the mandatory input fine grid layer height/pressure files).

Two types of input files must be supplied for each fine grid nest, while all others are optional. The mandatory files are the gridded height/pressure and area emissions files. The optional files include gridded landuse, winds, and vertical diffusivities. If any of the optional files are not supplied, CAMx interpolates the missing fields, as well as all other necessary gridded data (temperature, moisture, etc.), from the coarse grid.

POLLUTANT REMOVAL

CAMx optionally treats the dry and wet removal of all modeled gaseous species. Dry deposition of gases is treated as a first-order removal process, in which a deposition velocity is calculated and used to determine the flux of pollutants from layer 1 to the ground. This removal flux is used as the lower boundary condition in the vertical diffusion algorithm. Dry deposition velocities are calculated using the seasonal/landuse dependent three-resistance approach of Wesley (1989), with some improvements following Kumar et al. (1996), and surface layer parameterizations of Louis (1979). The Wesely approach is heavily dependent on proper specification of Henry's Law solubility constants and an aqueous reactivity parameter. These and other species-dependent values are supplied to CAMx for all CBM-IV species via the chemistry parameters file. Gridded landuse is supplied to the coarse grid and optionally any fine grids; season is determined by the simulation date.

Wet scavenging of gases is treated using a scavenging coefficient approach of Maul (1980) as implemented in CALPUFF (EPA, 1995). In this approach the fraction of pollutant mass removed from a given cell is an exponential function of a species-dependent scavenging coefficient and time step length. The scavenging coefficient is a function of Henry's Law solubility and rainfall rate. Gridded hourly rainfall rates (in/hr) must be supplied to CAMx if the wet deposition option is invoked.

PLUME-IN-GRID (PiG) SUBMODEL

Even with nested-grids there are lower limits on the grid size. Practical and theoretical considerations suggest that the lower limit is about 1000 meters. However, finer resolution may sometimes be needed to adequately model the chemistry of point source NO_x plumes. To deal with subgrid scale processes, CAMx incorporates a Plume-in-Grid (PiG) feature which allows CAMx to track individual plume segments, accounting for dispersion and chemical evolution, until such time as their mass can be adequately represented within the grid model framework. CAMx contains a new PiG methodology aimed at treating large NO_x point sources

called the Greatly Reduced Execution and Simplified Dynamics (GREASD) PiG which is much faster and structurally simpler than other PiG versions.

A highly simplified schematic illustration of the CAMx GREASD PiG submodel is given in Figure 2-1. A stream of plume segment “puffs” is released from a selected NO_x point source for each model driving time step (an elevated point source is selected for PiG treatment by specifying a negative stack diameter). This stream may be represented by a single puff, or by several, depending upon the relationship between the wind speed at the height of final plume rise, and the user-defined maximum puff length. For a given maximum length, more puffs will be released in stronger wind conditions while as little as one puff will be released in lighter wind conditions. GREASD PiG is formulated in this way to avoid producing very long narrow puffs that may span several grid cells.

The guidance for selecting maximum puff length is to limit their length to about half the minimum grid cell size to be used in the simulation. For example, in a simulation using nested grids with a minimum cell size of 4 km, a maximum puff length should be set to 2 km. In the case of a single coarse grid at 20 km size, the maximum length could be between 5-10 km. It is recommended that puffs do not exceed about 10 km in length, regardless of grid cell size. On the other hand, since this parameter has a strong influence on the total number of puffs tracked on the grid, use of a very short maximum puff length will increase model computational requirements.

GREASD PiG puffs are assumed to possess a Gaussian shaped two-dimensional concentration distribution in cross-section, but a constant distribution length-wise. The Gaussian distribution is treated analytically, and not through the use of concentric shells. The height and width of each puff are defined independently in terms of the horizontal and vertical Gaussian standard deviations (σ_y and σ_z), respectively. The total cross-sectional width and depth both extend $\pm 1.5\sigma$ from puff centerline. The limits of $\pm 1.5\sigma$ result in a two-dimensional average concentration that about equals the uniformly mixed concentration assumption.

Each individual puff is moved horizontally downwind; currently, puffs do not move vertically and stay at a constant elevation above the ground throughout their lifetime. As they move downwind, they grow via diffusion and undergo certain chemical reactions. Puff growth in width and depth are treated semi-independently, but no growth is assumed to occur longitudinally. The growth increment of σ_z for a given puff is a function of the gridded vertical diffusion coefficient from the occupied cell, total puff age, and time step length. Growth in σ_y is similarly calculated, but using a scaled value of the vertical diffusion coefficient.

Chemistry is performed by assuming a uniform mass distribution throughout the entire puff (i.e., concentration of a given species is defined by puff mass divided by puff volume). Puff chemistry is highly simplified as only three reactions are treated: (1) the NO-NO termolecular reaction producing NO₂, (2) NO_x-O₃ equilibrium via titration, and (3) nitric acid formation via separate nighttime and daytime pathways. This approach allows for only four species to be carried: NO, NO₂, O₃, and HNO₃. Only ozone is entrained during the life of the puff, and all NO_x originates from initial emissions. As ozone is depleted, through any of the reactions described above, the depleted ozone mass is immediately removed from the host grid cell, thereby removing the need to carry parallel chemistry puffs that double PiG memory requirements. Kumar and Russell

(1996) found that a PiG model with simplified inorganic chemistry produced results that were very similar to full chemistry.

There are two schools of thought regarding the appropriate times at which to dump puff mass into the host model grid system. The first primarily focuses on the physical size of puffs relative to grid cells. It is assumed that once puffs are large enough to be adequately resolved by a grid, their mass should be added to the host cell. The two principle problems associated with this approach are deciding what the appropriate size criteria are to be, and how to distribute puff mass into the grid system. Almost always, puffs are super-resolved in the vertical long before their widths become commensurate with grid widths. The second school focuses on the chemical maturity of the puffs (Gillani and Pleim, 1996), and the potential performance effects of dumping immature plume mixtures into a grid system. The main problem seen with this approach relates to how chemically mature plume mixtures may be identified within an ever-evolving puff relative to an ever-evolving grid chemistry. Puffs may reach a stage of chemical maturity after very long simulation periods (say 24 hours), however it is unrealistic to assume that puffs will maintain physical coherence over such a long period given the cumulative effects of wind shears and mixing gradients. In summary, neither of the above approaches is completely satisfactory and we strongly believe that further research is needed to develop new approaches to PiG modeling that adequately address both chemical maturity and physical size considerations.

The GREASD PiG dumping criteria is based upon the first approach described above that suggests that puffs should dump when adequately resolved by the grid. However, the CAMx approach acknowledges the problem of super-resolving puffs vertically by employing the following methodology. Puffs are allowed to grow unchecked until the depth defined by $\pm 1 \sigma_z$ spans the distance from the midpoint of the layer below the current host cell (or the ground) to the midpoint of the layer above. At this point, the puff is considered to be vertically resolved, and is limited to its current size. Puff NO_x and nitric acid masses are “leaked” from the puff in subsequent time steps at a rate that is linked to the rate at which σ_y and σ_z would have continued to grow given the current cell conditions. For a puff just reaching this state, the rate of mass leakage is small as the tails of the Gaussian distribution are cut off and leaked. As this puff ages further, the rate of leakage increases as the central portion of the Gaussian distribution grows outwards toward the fixed puff edge and material from the central portion of the Gaussian distribution is cut off and leaked.

Puffs are “slaughtered” (meaning that all remaining mass is leaked to the host cell) once the puff NO_x concentration is reduced to below twice the cell NO_x concentration. Puffs are also slaughtered if they reach a user-specified maximum age (usually 12-24 hours). However, in an effort to prohibit the sudden introduction of much puff NO_x mass to the grid, the age-limited puffs are slaughtered by undergoing increased artificial leakage over a period of about 1-1.5 hours (depending on time step and puff size).

CHEMISTRY

Chemistry Solver

Numerically integrating (solving) the time evolution of the gas phase chemistry is typically the most “expensive” part of a photochemical grid model simulation for ozone (aerosol phase chemistry may be even more expensive but the discussion that follows is for gas-phase

simulation of ozone). For example, in the EPA UAM, the gas-phase chemistry consumes about 85% of the model CPU time. Thus, the efficiency of the chemistry solver is the dominant factor in determining the overall efficiency of a grid model. The most accurate solution methods available are the "Gear" type implicit solvers (Gear, 1971) such as LSODE (Hindmarsh, 1983). Gear solvers are stable when applied to "stiff" problems, such as gas phase chemistry, but they are impractically slow for grid model applications. Sun et al. (1993) developed an implicit-explicit hybrid (IEH) method based on LSODE that is accurate and moderately fast. However, the IEH method is not considered fast enough to use in CAMx for regional simulations (it is estimated that the IEH method would consume about 85% of the CPU time in CAMx simulations). Winkler, Chock and Sun (1995) evaluated several other widely used numerical methods against LSODE and IEH, but found that none of the methods that were faster than IEH were very accurate. Consequently, a new chemistry solver was developed for CAMx with two objectives: (1) increased efficiency and (2) increased flexibility (see the discussion of flexibility under chemical mechanism compiler, below).

The CAMx chemistry solver uses a hybrid numerical approach to solve the gas-phase chemistry. The fastest reacting species (the radicals) are solved using the steady state approximation, i.e., it is assumed that their concentrations are fully equilibrated to, and determined by, the slower reacting (state) species. This is a good approximation for the radicals because their chemical lifetimes are very short compared to the model timesteps. The solution for the radicals uses an implicit numerical method that accurately accounts for the strong couplings between radical species concentrations. Radicals are not transported by the model advection because their lifetimes are so short that transport is negligible. Rather, the radicals are re-calculated at equilibrium with the remaining (state) species each time chemistry is performed. The state species are divided into two group: fast state species with chemical lifetimes comparable to model timesteps, and slow state species with chemical lifetimes much longer than model time steps. The fast state species are solved using a second order implicit Runge-Kutta method (see, for example, Lambert, 1973) and the slow state species are solved explicitly. If necessary, chemistry time steps are sub-divided for the solution of the fast state species to obtain an accurate solution. The solutions for the radicals and slow state species are continually updated to remain synchronous with the solution of the fast state species.

The species NO, NO₂, and O₃ are always considered fast state species. PAN is either considered fast or slow depending upon whether it's concentration is greater or less than 1% of NO₂, respectively. Since the number of fast species is variable based on the chemical condition, this method is referred to as an "adaptive hybrid method" (Guthrie et al., 1995).

Chemical Mechanism Compiler

A practical limitation of many chemistry solvers for photochemical grid models has been that the solver is coded by hand for a single mechanism. This means that any non-trivial change to the mechanism requires time consuming manual re-coding of the solver followed by careful testing to assure that the re-coding is free of errors. To overcome this limitation, the CAMx chemistry solver is prepared by a pre-processor program called the Chemical Mechanism Compiler (CMC). The CMC reads an ASCII file that lists the reactions for the mechanism and then prepares FORTRAN subroutines that are ready to be linked into the CAMx chemistry solver. This automation means that changes to the mechanism can be made quickly and with a high degree of confidence that they are correctly implemented. Another advantage of this design is that several

mechanisms can be implemented in the model in parallel allowing the user to switch between mechanisms simply by changing a model input (the CHEMPARAM file, discussed below).

CMC Solver Evaluation

The accuracy of the CMC solver has been evaluated in a box model by comparison to results for a Gear solver (the Gear solver results are considered an accurate benchmark, as discussed above). The Gear solver used was LSODE. Results are shown in Figure 2-2 and 2-3 for two representative conditions:

- 1) An initial VOC:NO_x ratio of 3:1 with no emissions
- 2) An initial VOC:NO_x ratio of 14:1 with subsequent continuous emissions of VOC and NO_x also at a 14:1 ratio.

In both figures, the lines show the Gear solver result and the symbols show the CMC solver result. Results are shown for several key species that also represent the three groups of species used in the CMC solver: steady state, fast state and slow state species. NO, NO₂, and O₃ are important for ozone modeling and are treated as fast state species by the CMC solver; OH is equally important and is treated as a steady state species; FORM and ALD2 are important sources of radicals and are treated as slow state species by the CMC solver. Agreement for all species is excellent in both tests.

OZONE SOURCE APPORTIONMENT TECHNOLOGY (OSAT)

Photochemical grid models are used to develop VOC and/or NO_x emissions control strategies that are designed to achieve ozone air quality standards. Currently, the development of an ozone attainment strategy involves iteration through many photochemical grid model scenarios to identify the source regions and source categories contributing to the high ozone levels that must be controlled. Because not all permutations of controls can be analyzed and photochemical grid model simulations can be computationally demanding, there is potential for implementing controls on sources that contribute little to the high ozone levels or, conversely, not controlling sources that do contribute.

CAMx incorporates a technique developed by ENVIRON for determining the contribution of emissions from specified source categories, source regions, and times of day to the elevated ozone concentrations estimated by a photochemical grid model (Yarwood et al., 1996a). The modeling method, known as Ozone Source Apportionment Technology (OSAT), utilizes tracers to access information on photochemical ozone and precursor production/destruction to track the amount of ozone formed due to emissions from specified source/geographic/temporal categories, as well as initial and boundary conditions. It accounts not only for the presence of ozone precursors from a given source region at a given receptor location, but also accurately estimates the cumulative contribution to ozone production of those precursors while they were en-route to the receptor. OSAT also keeps track of when ozone production occurred under locally VOC- or NO_x-limited conditions, further aiding in the design of effective ozone control strategies. See the Ozone Tool User's Guide for a complete guide to the OSAT model as implemented in UAM-IV.

The software accesses normal internal CAMx information such as local NO_x , VOC and ozone production/destruction rates for use in tracer calculations external to the CAMx chemistry procedure. The CAMx formulations for transport and dispersion are extended to allow for the extra tracer species required by the source apportionment model. This approach ensures that the source apportionment and standard CAMx estimate identical ozone and precursor concentrations for the same scenario.

A distinct set of tracer species is used for each user-specified source area. Some tracers represent the potential presence and dilution of precursors from a specific source area and identify the transport time from release to any receptor (timing tracers). Other tracers represent the chemical decay of NO_x and VOC emissions from a specific source area plus the ozone formation activity attributable to those emissions (ozone reaction tracers). Source areas can be defined in terms of geographical areas, emissions categories (e.g., mobile, stationary, biogenic) and temporal release periods (e.g., morning vs. afternoon).

Timing Tracers

The first category of tracers are “timing” tracers; of which there are two types: inert and decay-companion tracers. Inert and decay-companion tracers are used in tandem to identify the times of emission releases impacting receptors. This method is much more computationally efficient than releasing non-decaying separate tracers for each of many short time periods, since with only two inert/decay-companion pairs per day per source area, temporal resolution equivalent to more than 50 separate non-decaying tracers per day per source area can be obtained.

Ozone Reaction Tracers

The second category of tracers are called “ozone-reaction” tracers. We use four “ozone-reaction” tracers per source grouping to account for the contributions of emissions from separate source groupings to the complex process of the ozone formation activity. The four “ozone-reaction” tracers are: a NO_x emission tracer (N), a VOC emission tracer (V), a tracer for ozone production attributed to NO_x emissions (O3N), and a tracer for ozone production attributed to VOC emissions (O3V). The O3V and O3N tracers are used to integrate the en-route contributions of NO_x and VOC emissions to ozone production/destruction activity. The emission rates of the N and V tracers are equal to the total NO_x and VOC emission rates for the source area, respectively.

As the N and V tracers are transported within the model, the N tracer mass chemically decays according to the local CAMx predicted NO_x destruction rates weighted by the fraction N_i/N_t (where N_i is the concentration of NO_x from source area i , and N_t is the total of NO_x concentration from all source areas). In the case of the V tracers, the reactivity of each V tracer (defined in terms of its average reaction rate with hydroxyl radical, KOH_i) is calculated in advance by averaging the OH rate constants of the speciated VOC emissions for its respective source region. At each CAMx time step, the V tracer mass decays at a rate estimated from the product of the local CAMx VOC decay rate and the reactivity weighted fraction V_i/V_t . O3N and O3V tracers for a particular source area accumulate a portion of the total ozone production/destruction activity that occurs in the CAMx grid cells where they reside at each chemistry time step.

The method allocates the ozone predicted by CAMx in any grid cell at any time across all emissions from all source regions and provides an indication of whether NO_x or VOC emissions control in each source area will be most effective in reducing that source region's contribution to ozone. Furthermore, analysis of the timing tracers provides an indication of what times of control will be most effective. *Note that the OSAT software can not quantify the magnitude of the ozone concentration response to reducing NO_x or VOC emissions in a particular source area; the only way to do this is to rerun CAMx with reduced emissions.*

VOC- versus NO_x-Limitation

The ability to determine whether ozone formation is locally limited by the availability of NO_x or VOCs is an important attribute of the OSAT methodology. The sensitivity of ozone formation to VOCs and NO_x at any given time is attributable to the fate of radicals. When NO_x is plentiful the main radical termination (i.e., HO_x removal) pathway is nitric acid formation, thus nitric acid (HNO₃) production is indicative of plentiful NO_x and VOC-limited ozone formation. When NO_x is scarce, radical-radical reactions dominate HO_x removal; thus, peroxide formation (H₂O₂ = hydrogen peroxide, or ROOH = organic hydroperoxides) is indicative of scarce NO_x and NO_x-limited ozone formation. Sillman (1995) has exploited this situation to develop useful indicators of VOC vs. NO_x limited ozone formation based on the ratio of peroxide production to nitric acid production. He proposed that the transition between these conditions occurs when:

$$P_{H_2O_2} / P_{HNO_3} = 0.35$$

where P_{HNO_3} and $P_{H_2O_2}$ are the production rates of nitric acid and hydrogen peroxide, respectively. In other words, when this ratio exceeds 0.35 ozone formation is NO_x-limited, and when this ratio is less than 0.35 ozone formation is VOC-limited. We use Sillman's indicator in the CAMx ozone source apportionment module to assess local VOC- or NO_x-limitations to ozone formation.

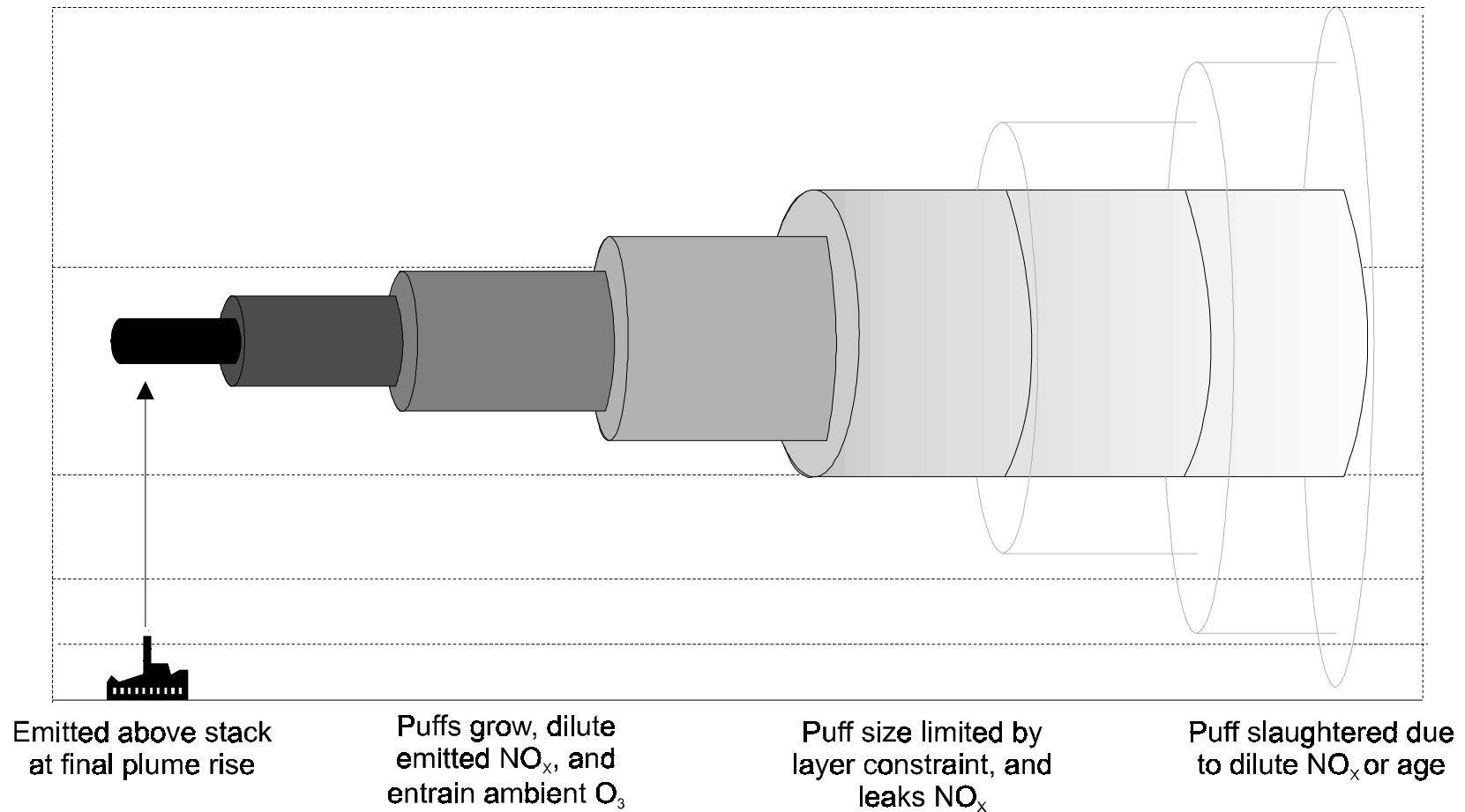


Figure 2-1. A simplified schematic representation of the CAMx GREASD PiG submodel. CAMx layers are shown by the horizontal dashed lines, CAMx grids are not shown. Puffs grow as they are transported downwind of the source. Puff growth is constrained when the puff depth reaches the layer thickness; the puff mass that exists between the constrained and unconstrained volumes is released to the grid.

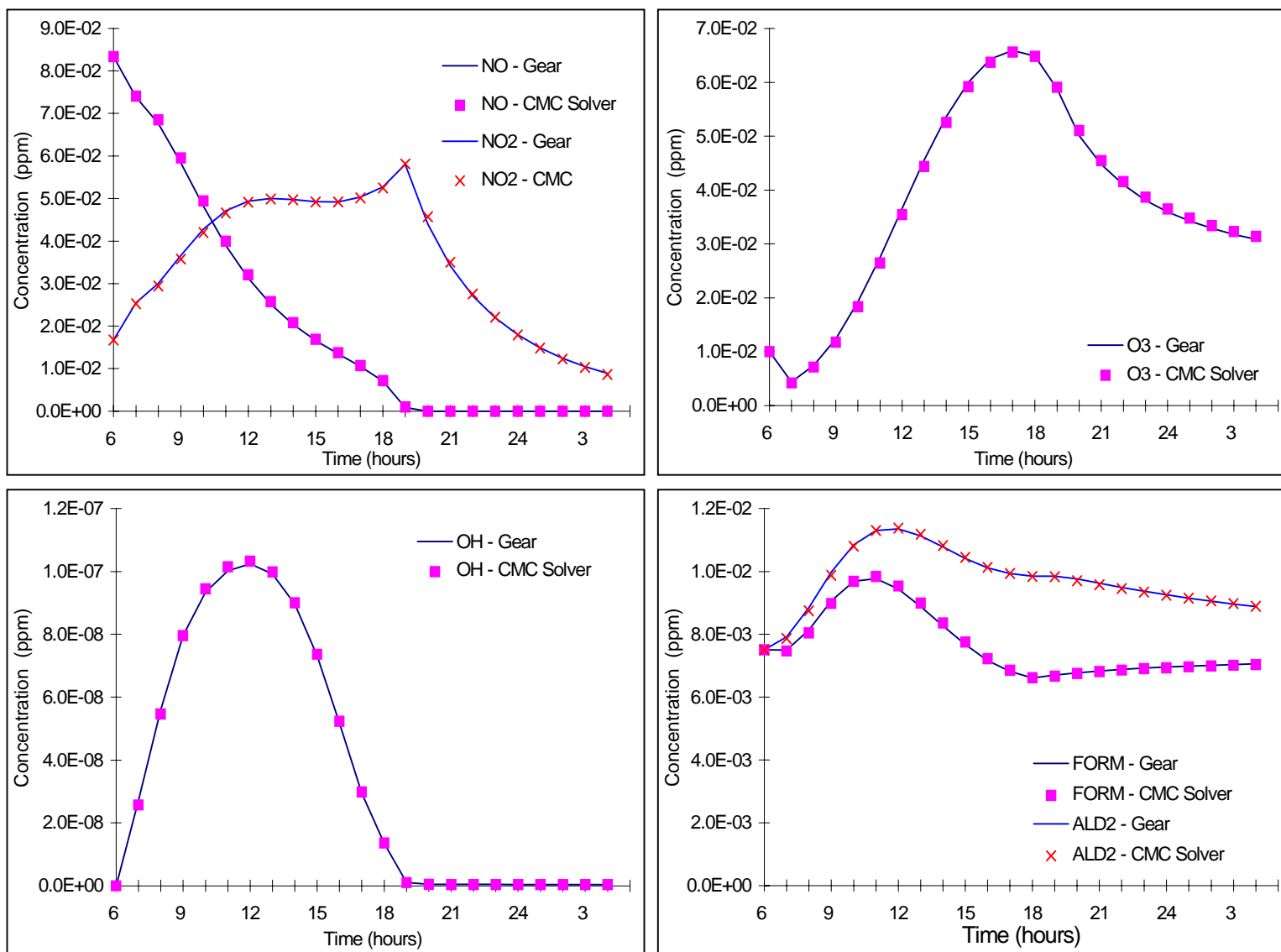


Figure 2-2. Comparison of CMC solver and Gear solver (LSODE) results for VOC:NO_x ratio of 3:1 with no emissions.

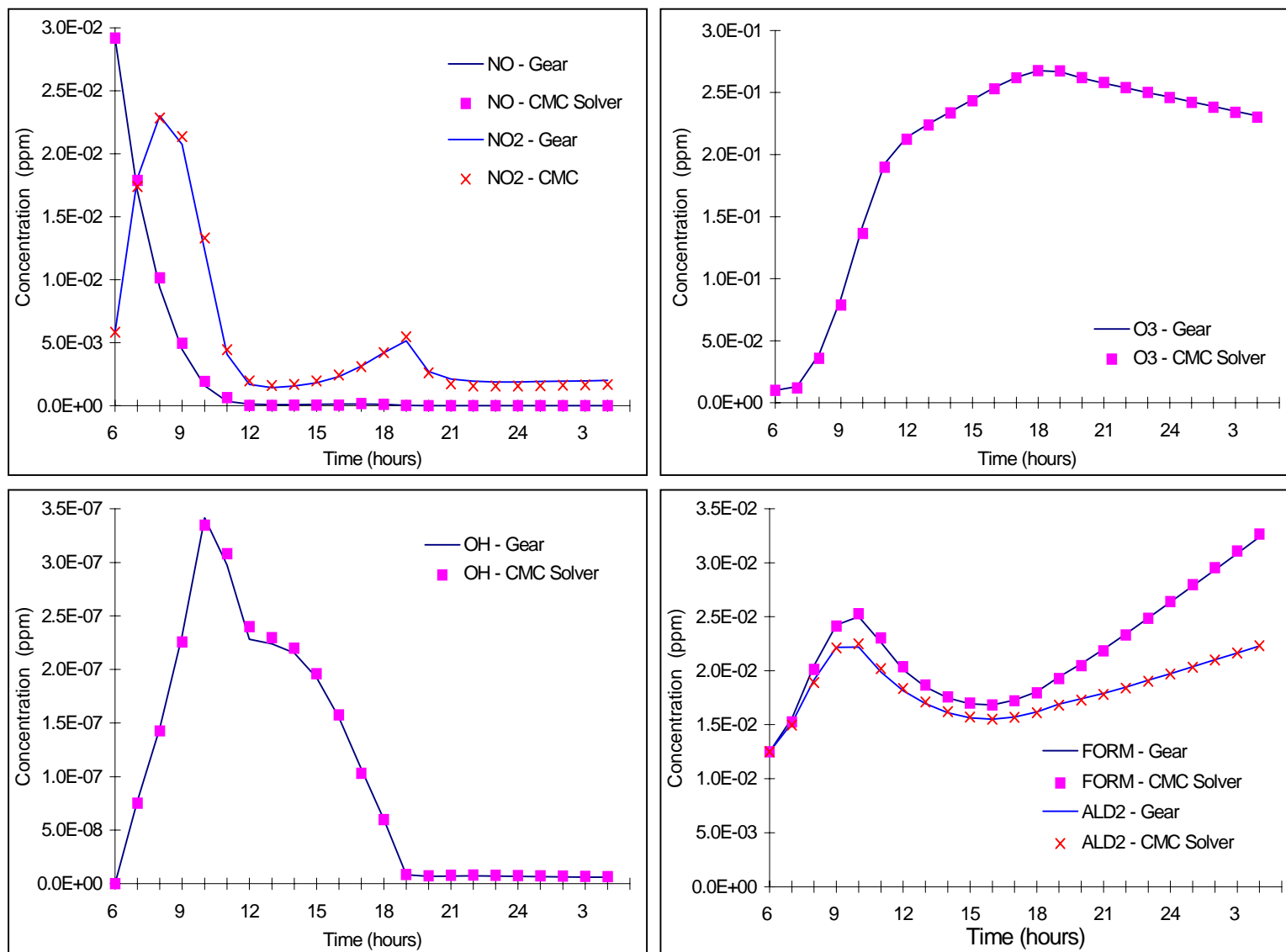


Figure 2-3 Comparison of CMC solver and Gear solver (LSODE) results for VOC:NO_x ratio of 14:1 with continuous emissions.

3. CAMx INPUT AND OUTPUT

CAMx requires inputs of radiative-chemical conditions and gridded inputs of surface characteristics, initial/boundary conditions, emission rates, and various meteorological measures over the entire modeling domain. Preparing this information requires several preprocessing/premodeling steps to translate “raw” emissions, meteorological, air quality and other data into final input files to CAMx. We expect that most CAMx applications will utilize output from a prognostic meteorological model that can generate all of the required four dimensional meteorological fields. Except for the chemistry parameters and run control files, CAMx is designed to read and write files with formats equivalent to UAM-V so that no manipulation of preexisting UAM-V inputs are required to run CAMx, and output files may be post-processed with software that the user may already possess. In any case, the most successful and technically defensible simulations using CAMx are those supported by enhanced emission, meteorological, and air quality monitoring programs. Table 3-1 summarizes the input data requirement of CAMx.

CAMx produces gridded hourly (or some other user specified time interval) average concentration output files containing either layer 1 fields or entire three-dimensional fields of user-selected species. An average output file is written for the coarse grid separately from one file containing all fine grid nests together. Gridded instantaneous fields of all species are assumed to be used for restarts only, and so only the last two hours are written to these files. Commonly available graphical output visualization and animation software can be applied for visualization of CAMx output files. The CAMx OSAT option outputs sufficient information to determine the emission regions, categories, times, and types (VOC or NO_x) that contribute to high ozone concentrations (see the Ozone Tool User's Guide). Diagnostic output files include several general files that track computer resources, repeat input selections, provide mass budget and diagnostic summaries, and provide error/warning messages.

CAMx RUN CONTROL FILE

The CAMx reads a run control file named “CAMx.in” that must exist locally in the directory from which the model is run. On computer platforms running UNIX the generation of the run control file is most easily accomplished in the job script that actually runs the model; Figure 3-1 shows an example of a CAMx job script that builds a “CAMx.in” file and runs the model for each day to be simulated. Alternatively, the run control file could be written separately with a name specific to a given simulation, then linked or copied to the standard “CAMx.in” filename before the model is executed at a command line or in a job script.

Table 3-2 provides all the information necessary to build a run control file. Some CAMx input files are not mandatory (e.g., rain, some fine grid files, etc.), but a record must exist as a place holder for their file names whether they are specified or not. Such records are indicated in Table 3-2 by noting that they are “NOT MANDATORY” in the description. Some are optional records, as selected by certain logical flag inputs, as shown in Table 3-2 by a check in the last column: if the option is not invoked these records should not appear in the file.

The first record of the run control file is a 60-character simulation message that is written to the headers of all UAM-type concentration output files. The second record is where the user

specifies a "root" path and filename that will be used for all standard CAMx output files. OSAT output uses a separate root filename specified in the OSAT section of the control file. The model appends suffixes to these root names according to the file type generated. The relationship between CAMx and OSAT suffix and file type is shown in Table 3-3

The CAMx allows for simulation start and end dates to be specified in either julian or calender formats; the model uses julian dates internally. All times must be given in military format (e.g., 1 PM must be given as 1300). Grid coordinates may be selected as UTM or latitude/longitude, but if the latter is selected, CAMx expects negative values for western longitudes. The chemistry parameters file format is unique to CAMx; a sample is given in Figure 3-2.

CAMx CHEMISTRY PARAMETERS FILE

The chemistry parameters file provides chemical information for the simulation and selects which mechanism is to be used by the CMC chemistry solver. An example file is shown in Figure 3-3 and the formats are defined in Table 3-4. CAMx checks that certain properties of the selected mechanism are consistent with parameters supplied on the input file (e.g., number of reactions, photolysis reactions and species). If any discrepancies are found, they are reported in the "diag" output file and the simulation is halted.

Gas Phase Chemistry

The chemical mechanisms supported in the current version of CAMx are all based on the Carbon Bond mechanism version 4 (CBM4; Gery et.al., 1989). However, the CMC could equally well be used to implement other mechanisms into CAMx, such as SAPRC (Carter, 1990). The mechanisms currently supported are described in Table 3-5 and a listing of the third mechanism is given in Table 3-6.

Mechanism 1 is provided for compatibility with the EPA regulatory version of UAM-IV, but it is not recommended for regional modeling applications because the radical termination reactions for XO₂, XO₂N and CRO are inadequate for NO_x-limited conditions. Mechanism 2 or 3 should be selected for regional modeling; the choice between 2 and 3 depends upon whether the user wishes to use the original isoprene chemistry or the newer (less reactive) Carter isoprene chemistry.

Mechanisms 1-3 are all balanced for nitrogen conservation so that predicted NO_y can be calculated as the sum of NO, NO₂, PAN, PNA, HONO, HNO₃, NTR and NXOY. NTR is the nitrogen in organic nitrates, and NXOY is the nitrogen in NO₃ and N₂O₅.

Aerosol Chemistry

The CAMx has been designed with model structures in place to handle aerosol chemistry, and so the chemistry parameters file defines the number of aerosol species (NAERO) and key physical properties for those species. Aerosol chemistry is not described in this version of the User's Guide, and user's should set NAERO to zero.

SETTING MODEL PARAMETERS

Important model parameters (e.g., maximum grid dimensions) are set in the "camx.prm" file. An example file is shown in Figure 3-3. Parameters that may need to be re-set according to the model application are:

mxcol	- the maximum number of columns of cells (left to right).
mxrow	- the maximum number of rows of cells (top to bottom).
mxlay	- the maximum number of vertical layers.
mxgrid	- the maximum number of grids including the mother grid and all nests.
mxld	- the larger value of mxcol or mxrow.
mxchdn	- the maximum number of grids nested below any one "parent" grid.
mxptsrc	- the maximum number of point sources.
mxpig	- the maximum number of PiG "puffs" that can be active in a simulation.

All of the above parameters can be determined before starting a simulation except for mxpig. If mxpig is exceeded during a simulation, the model will halt: simply increase mxpig and restart the simulation if this happens.

The other parameters in this file will not normally need to be changed and are not discussed further.

CAMx OUTPUT FILES

Coarse and fine grid instantaneous files contain full three-dimensional fields of all species modeled, while the coarse and fine grid average files contain only those species specified in the run control file. For flexibility, CAMx offers the option to write full three-dimensional average concentration fields, or just layer 1 two-dimensional fields (see the "3-D average file" option in Table 3-2). It is permissible to change the number of species on the average file, or change between 2-D and 3-D average files, from one CAMx simulated day to the next (provided the days are configured as separate CAMx runs). As the instantaneous concentration files are used primarily for CAMx restart capabilities, the model only writes instantaneous fields for the latest two simulation hours. The instant file labeled "1" receives average fields for the latest odd hour, and the file labeled "2" receives fields for the latest even hour. PiG output files are unique to CAMx.

Options for Format of Binary Input/Output Files

CAMx reads and writes many 3-D, time resolved files that require significant disk storage. To minimize the storage requirements, these files are in binary formats. Most UNIX workstations use the same binary format (IEEE, big endian). Digital Equipment Corporation (DEC) Alpha workstations use a different format by default. This can be changed by invoking a DEC compiler option "-convert big_endian." However, because of the way some variables (e.g., species names) are stored in the binary formatted files, files written on a DEC Alpha workstation with the "convert big_endian" option are not readable by other workstations. Engineers from DEC have provided a routine to solve this problem (BSWAP), and it is provided with the CAMx source code. DEC Alpha users who wish to exchange binary files with other work stations can compile

CAMx with the Makefile provided for DEC Alpha workstations that calls the routine "BSWAP.CVT.F" and invokes the compiler option "-convert big_endian." Users of other workstations should use a Makefile that links in the dummy routine "BSWAP.NOCVT.F" which performs no conversion.

OSAT

A description of the options and file formats for OSAT is provided in the User's Guide to the Ozone Tool: Ozone Source Apportionment Technology for UAM-IV (Yarwood et.al., 1996b). The implementations of OSAT in UAM-IV and CAMx are very similar, and the information in the Ozone Tool User's Guide combined with the sample job script in Figure 3-1 will enable CAMx user's to use and understand all of the OSAT features. The OSAT description will be fully integrated into the CAMx user's guide in the next version due later this year.

Table 3-1. Data Requirements of CAMx

DATA CLASS	DATA TYPES
Meteorological Supplied by a Meteorological Model	3-Dimensional Gridded Fields Winds Temperatures Vertical Diffusivity Pressure Water Vapor Cloud Cover Rainfall
Air Quality Obtained from Measured Ambient Data	Gridded Initial Concentrations Hourly Gridded Boundary Concentrations Time/space Constant Top Concentrations
Emissions Supplied by an Emissions Model	Elevated Point Sources Gridded Sources Low-level Point Mobile Anthropogenic Area Biogenic Area
Geographic Supplied by USGS Landuse Maps	Gridded Land Use/Surface Cover Gridded Surface UV Albedo codes
Other Ozone column from TOMS data Photolysis rates from radiative model	Vertical Grid Structure Atmospheric radiative properties Gridded haze codes Gridded ozone column codes Photolysis rates lookup table

Table 3-2. Description of the CAMx run control file (CAMx.in)

Record Label	Format	Description	Record Required	Record Optional
<user input>	A60	Simulation message (to be written to concentration file headers)	✓	
Root output name	20X, A80	Root output path/filename (see Table 3-3 for description of file suffixes)	✓	
Start time/date	20X, *	Simulation start time (midnight = 0, 1 PM = 1300) Simulation start date (Julian = YYJJJ, Calendar = YYMMDD)	✓	
End time/date	20X, *	Simulation end time (midnight = 2400, 1 PM = 1300) Simulation end date (Julian = YYJJJ, Calendar = YYMMDD)	✓	
DT:max,in,emis out	20X, *	Maximum allowable time step (hours) Input frequency of input environmental fields (hours) Input frequency of input emissions (hours) Output frequency (hours)	✓	
nx,ny,nz	20X, *	Number of coarse grid columns Number of coarse grid rows Number of coarse grid layers	✓	
xorg,yorg,dx,dy	20X, *	Longitudinal origin of coarse grid (UTM = km, W lon = -deg) Latitudinal origin of coarse grid (UTM = km, N lat = deg) Coarse grid longitudinal spacing (UTM = km, lon = deg) Coarse grid latitudinal spacing (UTM = km, lat = deg)	✓	
time zone, UTM zone	20X, *	Time zone (Eastern = 5, Central = 6, Mountain = 7, Pacific = 8) UTM zone	✓	
PiG parameters	20X, *	Maximum PiG puff length (m) Maximum PiG puff age (hours)	✓	
Avg output species	20X, *	Number of species to be written to average output file (NAVG)	✓	

Table 3-2. Description of the CAMx run control file (CAMx.in)

Record Label	Format	Description	Record Required	Record Optional
		If NAVG>0, repeat this record for each set of 6 species		
	20X, 6A10	Species names to be written to average output file		✓
# of fine nests	20X, *	Number of fine nested grids (NEST)	✓	
		If NEST>0, repeat this record for each find grid		
i1,i2,j1,j2,nz,mesh	20X, *	Longitudinal starting index (coarse grid cell) Longitudinal ending index (coarse grid cell) Latitudinal starting index (coarse grid cell) Latitudinal ending index (coarse grid cell) Number of fine grid layers Fine grid meshing factor		✓
Restart	20X, L10	Restart flag (false = read initial air quality file)	✓	
Chemistry	20X, L10	Chemistry flag (false = inert)	✓	
Dry dep	20X, L10	Dry deposition flag	✓	
Wet dep	20X, L10	Wet deposition flag	✓	
PiG submodel	20X, L10	PiG submodel flag	✓	
UTM cartesian grid	20X, L10	UTM Cartesian grid flag (false = lat/lon grid)	✓	
Staggered winds	20X, L10	Staggered (cell interface) input wind field flag (false = cell centered)	✓	
Treat area emiss	20X, L10	Area source flag	✓	
Treat point emiss	20X, L10	Point source flag	✓	
1-day emiss inputs	20X, L10	Date-insensitive emission inputs flag (false = checks file dates)	✓	

Table 3-2. Description of the CAMx run control file (CAMx.in)

Record Label	Format	Description	Record Required	Record Optional
3-D average file	20X, L10	3-D average output file (false = layer 1 concentrations only)	✓	
Source apportion	20X, L10	OSAT flag	✓	
		If the OSAT = TRUE, provide the next 8 records		
SA File Root	20X, A80	Root output path/filename for OSAT		✓
Technology type	20X, A80	The letters OSAT (other options will be available in the future)		✓
Crs, Fin sfc output	20X, *	Flags to write/omit surface output files for coarse and fine grids		✓
Stratify Boundary	20X, L10	Stratify boundary tracers flag (false = single tracer group for all boundaries)		✓
# of Source Regions	20X, *	Number of source regions (1 or greater)		✓
# of Source Groups	20X, *	Number of source groupings (1 or greater)		✓
Use leftover group	20X, L10	Use leftover group flag		✓
# timing releases	20X, *	Number of timing releases per day (may be zero)		✓
Chemparam	20X, A80	Input chemistry parameters path/filename	✓	
Photolysis rates	20X, A80	Input photolysis rates path/filename	✓	
Landuse	20X, A80	Input coarse grid landuse path/filename	✓	
Height/pressure	20X, A80	Input coarse grid height/pressure path/filename	✓	
Wind	20X, A80	Input coarse grid wind path/filename	✓	
Temperature	20X, A80	Input coarse grid temperature path/filename	✓	
Water vapor	20X, A80	Input coarse grid water vapor path/filename	✓	

Table 3-2. Description of the CAMx run control file (CAMx.in)

Record Label	Format	Description	Record Required	Record Optional
Cloud cover	20X, A80	Input coarse grid cloud cover path/filename	✓	
Rainfall	20X, A80	Input coarse grid rainfall path/filename (WETDEP = TRUE)	✓	
Vertical diffsvty	20X, A80	Input coarse grid vertical diffusivity path/filename	✓	
Initial conditions	20X, A80	Input coarse grid initial conditions path/filename (RESTART = FALSE)	✓	
Boundary conditions	20X, A80	Input coarse grid boundary conditions path/filename	✓	
Top concentration	20X, A80	Input coarse grid top boundary conditions path/filename	✓	
Albedo/haze/ozone	20X, A80	Input albedo/haze/ozone column path/filename	✓	
Point emiss	20X, A80	Input point source path/filename (POINT = TRUE)	✓	
Area emiss	20X, A80	Input coarse grid area source path/filename (AREA = TRUE)	✓	
		If NEST>0 and DRYDEP = TRUE, repeat this record for each fine grid		
Landuse Grd#n	20X, A80	Input fine grid landuse path/filename for grid n (NOT MANDATORY) ¹		✓
		If NEST>0, repeat this record for each fine grid		
Hght/press Grd#n	20X, A80	Input fine grid height/pressure path/filename for grid n		✓
		If NEST>0, repeat this record for each fine grid		
Wind Grd#n	20X, A80	Input fine grid wind path/filename for grid n (NOT MANDATORY) ¹		✓
		If NEST>0, repeat this record for each fine grid		
Vertical diff Grd#n	20X, A80	Input fine grid vertical diffusivity path/filename for grid n (NOT MANDATORY) ¹		✓

Table 3-2. Description of the CAMx run control file (CAMx.in)

Record Label	Format	Description	Record Required	Record Optional
If NEST>0, repeat at this record for each fine grid				
Area emiss Grd#n	20X, A80	Input fine grid area source path/filename for grid n		✓
If RESTART = TRUE provide this record				
Coarse grid restart	20X, A80	Coarse grid restart path/filename		✓
If RESTART = TRUE and NEST>0 , provide this record				
Fine grid restart	20X, A80	Fine grid restart path/filename		✓
If RESTART = TRUE and PiG = TRUE, provide this record				
PiG restart	20X, A80	PiG restart path/filename		✓
If the OSAT = TRUE, provide the next 2 records				
Source area mapping	20X, A80	OSAT, source area mapping path/filename		✓
Receptor definition	20X, A80	OSAT, receptor definition path/filename		✓
If OSAT = TRUE and RESTART = TRUE, provide the next 2 records				
CG tracer restart	20X, A80	OSAT, coarse grid tracer restart path/filename		✓
FG tracer restart	20X, A80	OSAT, fine grid tracer restart path/filename		✓

Table 3-2. Description of the CAMx run control file (CAMx.in)

Record Label	Format	Description	Record Required	Record Optional
		If OSAT = TRUE, repeat the next 2 records for the number of source groups or if using leftover group, the number of source groups minus 1. Provide the following record for each grid (NEST + 1)		
Area Grp#m grd#n	20X, A80	Input tracer area emissions path/filename for source group m and grid n (NOT MANDATORY) ¹		✓
Point Grp#m	20X, A80	Input tracer point source filename for source group m (NOT MANDATORY) ¹		✓

¹For records described as “NOT MANDATORY”, the user has the option to leave the filename blank. For example, if grid nests are selected, records are required for fine grid winds, but the user can leave the fine grid wind filename(s) blank causing CAMx to interpolate the fine grid winds from coarse grid winds.

Table 3-3. CAMx output file suffixes and their corresponding file types

Suffix	CAMx file type
.out	Simulation tracking file (CPU, mass budget, input files read, error/warning messages)
.diag	Simulation diagnostic file (repeat of run control inputs, PiG diagnostics, miscellaneous diagnostic output)
.mass	Mass budget file for subsequent postprocessing
.inst.1	Coarse grid binary instantaneous concentration file for last odd simulation hour (used for restarts)
.inst.2	Coarse grid binary instantaneous concentration file for last even simulation hour (used for restarts)
.finst.1	Fine grid binary instantaneous concentration file for last odd simulation hour (used for restarts)
.finst.2	Fine grid binary instantaneous concentration file for last even simulation hour (used for restarts)
.avrg	Coarse grid binary average concentration file; optionally contains 2-D layer 1 concentration field or full 3-D concentration field
.favrg	Fine grid binary average concentration file; optionally contains 2-D layer 1 concentration field or full 3-D concentration field
.pig	PiG submodel file (used for restarts)
Suffix	OSAT file type
.sa.inst.1	Coarse grid binary instantaneous concentration file for last odd simulation hour (used for restart)
.sa.inst.2	Coarse grid binary instantaneous concentration file for last even simulation hour (used for restart)
.sa.finst.1	Fine grid binary instantaneous concentration file for last odd simulation hour (used for restart)
.sa.finst.2	Fine grid binary instantaneous concentration file for last even simulation hour (used for restart)
.sa.surf	Coarse grid binary average concentration file; 2-D layer 1 concentration field
.sa.fsrf	Fine grid binary average concentration file; 2-D layer 1 concentration field
.sa.receptor	OSAT receptor average concentration file in ASCII format for the Microsoft Excel based receptor file "browser."

Table 3-4. Description of the CAMx chemistry parameters file.

Record Label	Format	Description	Record Required	Record Optional
Mechanism ID	20X, *	ID number of CMC solver mechanis,	✓	
Description	20X, A	Message record to describe this file	✓	
No of gas species	20X, *	Number of gas species (minimum of 2) NGAS	✓	
No of aero species	20X, *	Number of aerosol species (minimum of 0) NAEARO	✓	
No of reactions	20X, *	Number of reactions (minimum of 1) NREACT	✓	
Prim photo rxns	20X, *	Number and list of primary photolysis reactions (must match the photolysis rates input file), by the; reaction numbers (minimum of 1 reaction)	✓	
No of sec photo rxn	20X, *	Number of secondary photolysis reactions (minimum of 1 reaction)	✓	
ID, prim ID, scale	20X, *	Scaling relationships for secondary photolysis reactions. There are 3 values on each record: the ID of the secondary photo rxn, the ID of the primary photo rxn used for scaling, and the scale factor. Repeat the record for each secondary photo rxn (minimum of 1 record).	✓	
Species Records	A	Heading	✓	
Gas Spec.....	A	Heading	✓	
Number	5X, A10, 2E10.0, 3F10.0	Parameters for the gas species: name, lower bound concentration (ppm), Henry's law constant (M/atm), Henry's law constant temperature dependance (K), molecular diffusivity ratio, Wesley's reactivity parameter. Repeat the record for each gas species (1 to NGAS).	✓	
Aero Spec....	A	Heading: The next record only appears for NAEARO>0		✓
Number	5X, A10, E10.0, F10.0	Parameters for the aero species: name, lower bound concentration ($\mu\text{g}/\text{m}^3$), molecular weight (Daltons). Repeat the record for each aero species 1 to NAEARO.		✓
Reaction records	A	Heading	✓	

Record Label	Format	Description	Record Required	Record Optional
rate const.....	A	Heading	✓	
Number	5X, E10.0, E15.0	Rate constants for the gas phase reactions ($\text{ppm}^{-1} \text{ hour}^{-1}$) at 298k and temperature dependancies (K). Repeat the record for each reaction 1 to NREACT. For reactions identified as photolysis reactions above, the values are not used and may be set to zero.	✓	

Table 3-5. Mechanisms implemented in the CAMx CMC chemistry solver.

Mechanism I.D. Number	Description
1	The CBM4 as implemented in the EPA UAM
2	Mechanism 1 with revised radical termination reactions
3	Mechanism 2 with updated isoprene chemistry based on Carter (1996) as implemented for the Ozone Transport Assessment Group (OTAG) by Whitten et.al., (1996).

Table 3-6. Listing of CMC solver mechanism 3: CBM4 with updated radical termination reactions and Carter isoprene mechanism. Rate constraints have units ppm⁻ⁿ hr⁻¹.

Rxn No	Reactants		Products		Rate Constant	
					k (298)	E/R
1	NO2	=	1.000 NO	1.000 O	Phot Rxn	
2	O	=	1.000 O3		259400000	-1175
3	O3	NO	=	1.000 NO2	1598.4	1370
4	O	NO2	=	1.000 NO	825000	0
5	O	NO2	=	1.000 NO3	138540	-687
6	O	NO	=	1.000 NO2	146280	-602
7	NO2	O3	=	1.000 NO3	2.8386	2450
8	O3		=	1.000 O	Phot Rxn	
9	O3		=	1.000 O1D	Phot Rxn	
10	O1D		=	1.000 O	2.55E+13	-390
11	O1D	H2O	=	2.000 OH	19560000	0
12	O3	OH	=	1.000 HO2	6000	940
13	O3	HO2	=	1.000 OH	179.94	580
14	NO3		=	0.890 NO2	0.890 O	0.110 NO
15	NO3	NO	=	2.000 NO2	2650000	-250
16	NO3	NO2	=	1.000 NO	1.000 NO2	35.406
17	NO3	NO2	=	1.000 N2O5	111180	-256
18	N2O5	H2O	=	2.000 HNO3	0.000114	0
19	N2O5		=	1.000 NO3	1.000 NO2	166.56
20	NO	NO	=	2.000 NO2	0.009234	-530
21	NO	NO2	=	2.000 HNO2	9.6E-09	0
22	NO	OH	=	1.000 HNO2	587940	-806
23	HNO2		=	1.000 NO	1.000 OH	Phot Rxn
24	OH	HNO2	=	1.000 NO2	586200	0
25	HNO2	HNO2	=	1.000 NO	1.000 NO2	0.0009
26	NO2	OH	=	1.000 HNO3	1009000	-713
27	OH	HNO3	=	1.000 NO3	13074	-1000
28	HO2	NO	=	1.000 OH	1.000 NO2	736200
29	HO2	NO2	=	1.000 PNA	0	0
30	PNA		=	1.000 HO2	1.000 NO2	0
31	OH	PNA	=	1.000 NO2	0	0
32	HO2	HO2	=	1.000 H2O2	248640	-1150
33	HO2	HO2	=	1.000 H2O2	13.086	-5800
34	H2O2		=	2.000 OH	Phot Rxn	
35	OH	H2O2	=	1.000 HO2	151200	187
36	OH	CO	=	1.000 HO2	19320	0
37	FORM	OH	=	1.000 HO2	1.000 CO	900000
38	FORM		=	2.000 HO2	1.000 CO	Phot Rxn
39	FORM		=	1.000 CO	Phot Rxn	
40	FORM	O	=	1.000 OH	1.000 HO2	1.000 CO
41	FORM	NO3	=	1.000 HNO3	1.000 HO2	1.000 CO
42	ALD2	O	=	1.000 C2O3	1.000 OH	38160

Rxn No	Reactants		Products		Rate Constant			E/R
					k(298)			
43	ALD2	OH	=	1.000 C2O3			1440000	-250
44	ALD2	NO3	=	1.000 C2O3	1.000 HNO3		222	0
45	ALD2		=	1.000 FORM	2.000 HO2	1.000 CO	Phot Rxn	
				1.000 XO2				
46	C2O3	NO	=	1.000 FORM	1.000 NO2	1.000 HO2	1692000	180
				1.000 XO2				
47	C2O3	NO2	=	1.000 PAN			822000	-380
48	PAN		=	1.000 C2O3	1.000 NO2		1.524	13500
49	C2O3	C2O3	=	2.000 FORM	2.000 XO2	2.000 HO2	222000	0
50	C2O3	HO2	=	0.790 FORM	0.790 XO2	0.790 HO2	576000	0
				0.790 OH				
51	OH		=	1.000 FORM	1.000 XO2	1.000 HO2	1260	1710
52	PAR	OH	=	0.870 XO2	0.130 XO2N	0.110 HO2	72180	0
				0.110 ALD2	-0.110 PAR	0.760 ROR		
53	ROR		=	0.960 XO2	1.100 ALD2	0.940 HO2	8226000	8000
				-2.100 PAR	0.040 XO2N			
54	ROR		=	1.000 HO2			5727000	0
55	ROR	NO2	=	1.000 NTR			1320000	0
56	O	OLE	=	0.630 ALD2	0.380 HO2	0.280 XO2	355200	324
				0.300 CO	0.200 FORM	0.020 XO2N		
				0.220 PAR	0.200 OH			
57	OH	OLE	=	1.000 FORM	1.000 ALD2	-1.000 PAR	2520000	-504
				1.000 XO2	1.000 HO2			
58	O3	OLE	=	0.500 ALD2	0.740 FORM	0.220 XO2	1.08	2105
				0.100 OH	0.330 CO	0.440 HO2		
				-1.000 PAR				
59	NO3	OLE	=	0.910 XO2	1.000 FORM	0.090 XO2N	681	0
				1.000 ALD2	1.000 NO2	-1.000 PAR		
60	O	ETH	=	1.000 FORM	1.700 HO2	1.000 CO	64800	792
				0.700 XO2	0.300 OH			
61	OH	ETH	=	1.000 XO2	1.560 FORM	0.220 ALD2	715200	-411
				1.000 HO2				
62	O3	ETH	=	1.000 FORM	0.420 CO	0.120 HO2	0.162	2633
63	TOL	OH	=	0.440 HO2	0.080 XO2	0.360 CRES	549000	-322
				0.560 TO2				
64	TO2	NO	=	0.900 NO2	0.900 HO2	0.900 OPEN	720000	0
				0.100 NTR				
65	TO2		=	1.000 CRES	1.000 HO2		15000	0
66	OH	CRES	=	0.400 CRO	0.600 XO2	0.600 HO2	3660000	0
				0.300 OPEN				
67	CRES	NO3	=	1.000 CRO	1.000 HNO3		1950000	0
68	CRO	NO2	=	1.000 NTR			1200000	0
69	OPEN		=	1.000 C2O3	1.000 HO2	1.000 CO	Phot Rxn	
70	OPEN	OH	=	1.000 XO2	2.000 CO	2.000 HO2	2640000	0
				1.000 C2O3	1.000 FORM			

Rxn No	Reactants			Products				Rate Constant		E/R
								k (298)		
71	OPEN	O3	=	0.030 ALD2	0.620 C2O3	0.700 FORM	0.9		500	
				0.030 XO2	0.690 CO	0.080 OH				
				0.760 HO2	0.200 MGLY					
72	OH	XYL	=	0.700 HO2	0.500 XO2	0.200 CRES	2172000		-116	
				0.800 MGLY	1.100 PAR	0.300 TO2				
73	OH	MGLY	=	1.000 XO2	1.000 C2O3		1560000		0	
74	MGLY		=	1.000 C2O3	1.000 HO2	1.000 CO	Phot Rxn			
75	O	ISOP	=	0.750 ISPD	0.500 FORM	0.250 XO2	3192000		0	
				0.250 HO2	0.250 C2O3	0.250 PAR				
76	OH	ISOP	=	0.912 ISPD	0.629 FORM	0.991 XO2	8856000		0	
				0.912 HO2	0.088 XO2N					
77	O3	ISOP	=	0.650 ISPD	0.600 FORM	0.200 XO2	1.14		0	
				0.066 HO2	0.266 OH	0.200 C2O3				
				0.150 ALD2	0.350 PAR	0.066 CO				
78	NO3	ISOP	=	0.200 ISPD	0.800 NTR	1.000 XO2	59760		0	
				0.800 HO2	0.200 NO2	0.800 ALD2				
				2.400 PAR						
79	XO2	NO	=	1.000 NO2			720000		0	
80	XO2	XO2	=				120000		-1300	
81	XO2N	NO	=	1.000 NTR			720000		0	
82	SO2	OH	=	1.000 SULF	1.000 HO2		66600		-160	
83	SO2		=	1.000 SULF			0.0049		0	
84	MEOH	OH	=	1.000 FORM	1.000 HO2		96000		0	
85	ETOH	OH	=	1.000 HO2	1.000 ALD2		258000		-176	
86	XO2	HO2	=				534000		-1300	
87	XO2N	HO2	=				534000		-1300	
88	XO2N	XO2N	=				120000		-1300	
89	XO2	XO2N	=				240000		-1300	
90	OH	HO2	=				9756000		-250	
91	CRO		=				0.016667		0	
92	OH	ISPD	=	1.565 PAR	0.167 FORM	0.713 XO2	2980000		0	
				0.503 HO2	0.334 CO	0.168 MGLY				
				0.273 ALD2	0.498 C2O3					
93	O3	ISPD	=	0.114 C2O3	0.150 FORM	0.850 MGLY	0.63		0	
				0.154 HO2	0.268 OH	0.064 XO2				
				0.020 ALD2	0.360 PAR	0.225 CO				
94	NO3	ISPD	=	0.357 ALD2	0.282 FORM	1.282 PAR	88.68		0	
				0.925 HO2	0.643 CO	0.850 NTR				
				0.075 C2O3	0.075 XO2	0.150 HNO3				
95	ISPD		=	0.333 CO	0.067 ALD2	0.900 FORM	Phot Rxn			
				0.832 PAR	1.033 HO2	0.700 XO2				
				0.967 C2O3						
96	NO2	ISOP	=	0.200 ISPD	0.800 NTR	1.000 XO2	0.0132		0	
				0.800 HO2	0.200 NO	0.800 ALD2				
				2.400 PAR						

```

#   Script to Run CAMx
#
set verbose
#
set INPUT   = "/disk9/camx/inputs"
set EMIS    = "/disk10/camx/emiss"
set PTRSCE  = "/disk10/camx/ptrsce"
set OUTPUT  = "/disk7/camx/outputs"
set TRACIN  = "/disk9/camx/osat/inputs"
set TRACOUT = "/disk7/camx/osat/outputs"
set TRACEMS = "/disk10/camx/osat/emiss"
#
date
#
#
#   --- Create the input file (always called CAMx.in)
#
cat << ieof > CAMx.in
CAMx OTAG BasD July 7, 1995 -- OSAT cem1A run11
Root output name |$OUTPUT/CAMx.070707.cem1A.run11
Start time/date  |0. 950707
End time/date    |2400. 950707
DT:max,in,emis,out|0.5 1. 1. 1.
nx,ny,nz         |64 63 5
xorg,yorg,dx,dy  |-99. 26. .5 .33333
time zone,UTM zone|6 16
PiG parameters   |5000. 12.
Avg output species|15
                  |NO          NO2          O3          PAR          TOL          ETH
                  |OLE          PAN          ISOP         XYL          FORM         ALD2
                  |HNO3         NXOY         NTR
# offline nests  |1
il,i2,j1,j2,nz,mesh|15 59 19 54 7 3
Restart          |false
Chemistry        |true
Dry dep          |true
Wet dep          |true
PiG submodel     |true
UTM cartesian grid|false
Staggered winds  |true
Treat area emiss |true
Treat point emiss|true
1-day emiss inputs|true
3-D average file |false
Source Apportion |true

```

Figure 3-1. A sample CAMx job script that generates a “CAMx.in” file and runs the model. This run has OSAT enabled with 19 source regions and 3 emission groups.

```

SA File Root      |$TRACOUT/CAMx.070707.cem1A.run11
Technology type   |OSAT
Crs,Fin sfc output|T T
Stratify Boundary|FALSE
# of Source Regions|19
# of Source Groups|3
Use leftover group|TRUE
# timing releases|0
Chemparam         |/models/camx/inputs/CAMx.chemparm.3
Photolysis rates  |$INPUT/rate.ng.99jul95.ai.basD
Landuse           |$INPUT/surf.cc.commonfile.ai.basD
Height/pressure   |$INPUT/rams/hght.cc.07jul95.ne.rams1b
Wind              |$INPUT/rams/wind.cc.07jul95.ne.rams1b
Temperature       |$INPUT/rams/tmpr.cc.07jul95.ne.rams1b
Water vapor       |$INPUT/rams/wvap.cc.07jul95.ne.rams1b
Cloud cover       |$INPUT/clou.cc.07jul95.ld.basD
Rainfall          |$INPUT/anlrain.950707.out
Vertical diffsvty |$INPUT/rams/vdif.cc.07jul95.wi.rams1bnew
Initial conditions|$INPUT/init.cc.07jul95.ld.basD
Boundary conditions|$INPUT/bndr.cc.07jul95.ld.basD.a0
Top concentration |$INPUT/topc.ng.commonfile.ai.basD
Albedo/haze/ozone |$INPUT/ahoz.cf.99jul95.ld.basD
Point emiss       |$PTRSCE/ptrs.ng.07jul95-07.ag.07cem1A-run11
Area emiss        |$EMIS/emis.cc.07jul95-07.ag.07cem1A-run11
Landuse Grd #1    |$INPUT/surf.ff.commonfile.ai.basD
Hght/press Grd #1|$INPUT/rams/hght.ff.07jul95.ne.rams1b
Wind Grd #1       |$INPUT/rams/wind.ff.07jul95.ne.rams1b
Vrtcal diff Grd #1|$INPUT/rams/vdif.ff.07jul95.wi.rams1bnew
Area emiss Grd #1|$EMIS/emis.ff.07jul95-07.ag.07cem1A-run11
Source area mapping|$TRACIN/source.map.states
Receptor definition|$TRACIN/receptor.cities
Area Grp#1 Grd#1  |$TRACEMS/bio2.cc.07jul95-95
Area Grp#1 Grd#2  |$TRACEMS/bio2.ff.07jul95-95.ne
Point Grp#1       |
Area Grp#2 Grd#1  |$TRACEMS/utillowp.cc.07jul95-07.ag.07cem1A-run11
Area Grp#2 Grd#2  |$TRACEMS/utillowp.ff.07jul95-07.ag.07cem1A-run11
Point Grp#2       |$PTRSCE/utillptrs.ng.07jul95-07.ag.07cem1A-run11
ieof
#
# --- Execute the model ---
#
/bin/time /models/camx/src.v1.10/CAMx > CAMx.070707.run11.cem1A.out
#
date
#
# --- Loop over remaining days to be simulated
#

```

Figure 3-1. Continued. A sample CAMx job script that generates a “CAMx.in” file and runs the model. This run has OSAT enabled with 19 source regions and 3 emission groups.

```

foreach today (08 09 10 11 12 13 14 15 16 17 18)
set yesterday = `echo $today | awk '{printf("%2.2d",$1-1)}'`
set todote = `echo $today | awk '{printf("%2.2djul95",$1)}'`
date
#
#
# --- Create the input file (always called CAMx.in)
#
cat << ieof > CAMx.in
CAMx OTAG BasD July $today, 1995 -- OSAT cem1A run11
Root output name      |$OUTPUT/CAMx.0707$today.cem1A.run11
Start time/date        |    0. 9507$today
End time/date          |2400. 9507$today
DT:max,in,emis,out    |0.5 1. 1. 1.
nx,ny,nz               |64 63 5
xorg,yorg,dx,dy        |-99. 26. .5 .33333
time zone,UTM zone     |6 16
PiG parameters         |5000. 12.
Avg output species     |15
                        |NO          NO2          O3          PAR          TOL          ETH
                        |OLE          PAN          ISOP         XYL          FORM         ALD2
                        |HNO3         NXOY         NTR
# of fine nests        |1
i1,i2,j1,j2,nz,mesh   |15 59 19 54 7 3
Restart                |true
Chemistry              |true
Dry dep                |true
Wet dep                |true
PiG submodel           |true
UTM cartesian grid     |false
Staggered winds        |true
Treat area emiss       |true
Treat point emiss      |true
1-day emiss inputs     |true
3-D average file       |false
Source Apportion       |true
SA File Root           |$TRACOUT/CAMx.0707$today.cem1A.run11
Technology type        |OSAT
Crs,Fin sfc output     |T T
Stratify Boundary      |FALSE
# of Source Regions    |19
# of Source Groups     |3
Use leftover group     |TRUE
# timing releases      |0
Chemparm               |/models/camx/inputs/CAMx.chemparm.3

```

Figure 3-1. Continued. A sample CAMx job script that generates a “CAMx.in” file and runs the model. This run has OSAT enabled with 19 source regions and 3 emission groups.

```

Photolysis rates | $INPUT/rate.ng.99jul95.ai.basD
Landuse          | $INPUT/surf.cc.commonfile.ai.basD
Height/pressure  | $INPUT/rams/hght.cc.$todate.ne.rams1b
Wind             | $INPUT/rams/wind.cc.$todate.ne.rams1b
Temperature      | $INPUT/rams/tmpr.cc.$todate.ne.rams1b
Water vapor      | $INPUT/rams/wvap.cc.$todate.ne.rams1b
Cloud cover      | $INPUT/clou.cc.$todate.ld.basD
Rainfall         | $INPUT/anlrain.9507$today.out
Vertical diffsvty | $INPUT/rams/vdif.cc.$todate.wi.rams1bnew
Initial conditions
Boundary conditions | $INPUT/bndr.cc.$todate.ld.basD.a0
Top concentration  | $INPUT/topc.ng.commonfile.ai.basD
Albedo/haze/ozone  | $INPUT/ahoz.cf.99jul95.ld.basD
Point emiss       | $PTRSCE/ptrs.ng.$todate-07.ag.07cem1A-run11
Area emiss        | $EMIS/emis.cc.$todate-07.ag.07cem1A-run11
Landuse          Grd #1 | $INPUT/surf.ff.commonfile.ai.basD
Hght/press       Grd #1 | $INPUT/rams/hght.ff.$todate.ne.rams1b
Wind             Grd #1 | $INPUT/rams/wind.ff.$todate.ne.rams1b
Vrtcal diff      Grd #1 | $INPUT/rams/vdif.ff.$todate.wi.rams1bnew
Area emiss       | $EMIS/emis.ff.$todate-07.ag.07cem1A-run11
Coarse grid restart | $OUTPUT/CAMx.0707$yesterday.cem1A.run11.inst.2
Fine grid restart  | $OUTPUT/CAMx.0707$yesterday.cem1A.run11.finst.2
PiG restart       | $OUTPUT/CAMx.0707$yesterday.cem1A.run11.pig
Source area mapping | $TRACIN/source.map.states
Receptor definition | $TRACIN/receptor.cities
CG tracer restart  | $TRACOUT/CAMx.0707$yesterday.cem1A.run11.sa.inst.2
FG tracer restart  | $TRACOUT/CAMx.0707$yesterday.cem1A.run11.sa.finst.2
Area              Grp#1 Grd#1 | $TRACEMS/bio2.cc.$todate-95
Area              Grp#1 Grd#2 | $TRACEMS/bio2.ff.$todate-95.ne
Point             Grp#1 |
Area              Grp#2 Grd#1 | $TRACEMS/utillowp.cc.$todate-07.ag.07cem1A-run11
Area              Grp#2 Grd#2 | $TRACEMS/utillowp.ff.$todate-07.ag.07cem1A-run11
Point             Grp#2 | $PTRSCE/utillptrs.ng.$todate-07.ag.07cem1A-run11
ieof
#
# --- Execute the model ---
#
/bin/time /models/camx/src.v1.10/CAMx > CAMx.0707$today.run11.cem1A.out
#
date
#
end
#

```

Figure 3-1. Concluded. A sample CAMx job script that generates a “CAMx.in” file and runs the model. This run has OSAT enabled with 19 source regions and 3 emission groups.

```

Mechanism ID      | 3
Description       | CBM-IV / updated rad-rad rxns / Carter 1 product ISOP mech
No of gas species | 25
No of aero species | 0
No of reactions   | 96
Prim photo rxns   | 6 1 38 39 9 45 95
No of sec photo rxn | 6
ID, prim ID, scale | 8 1 0.053
                  | 14 1 33.9
                  | 23 1 0.1975
                  | 34 39 0.189
                  | 69 38 9.04
                  | 74 38 9.64

```

Species Records

	Gas Spec	lower bnd	H-law	T-fact	Difftrat	Reactivty
1	NO	1.00E-15	1.90e-03	-1480.	1.29	0.0
2	NO2	1.00E-09	1.00e-02	-2516.	1.60	0.1
3	O3	1.00E-09	1.10e-02	-2415.	1.63	1.0
4	PAN	1.00E-09	3.60e+00	-5910.	2.59	0.1
5	NXOY	1.00E-12	3.20e+04	-8706.	2.45	0.1
6	OLE	1.00E-09	5.00e-03	0.	1.80	0.0
7	PAR	1.00E-04	1.00e-03	0.	2.00	0.0
8	TOL	1.00E-09	1.20e+00	0.	2.26	0.0
9	XYL	1.00E-09	1.40e+00	0.	2.43	0.0
10	FORM	1.00E-09	6.30e+03	-6492.	1.29	0.0
11	ALD2	1.00E-09	6.30e+03	-6492.	1.56	0.0
12	ETH	1.00E-09	1.00e-02	0.	1.25	0.0
13	CRES	1.00E-09	2.70e+03	-6492.	2.45	0.0
14	MGLY	1.00E-09	2.70e+03	-6492.	2.00	0.0
15	OPEN	1.00E-12	2.70e+03	-6492.	2.47	0.0
16	PNA	1.00E-09	2.00e+04	-5910.	2.09	0.0
17	CO	1.00E-02	1.00e-10	0.	1.25	0.0
18	HONO	1.00E-09	5.90e+01	-4781.	1.62	0.1
19	H2O2	1.00E-09	7.40e+04	-6643.	1.37	1.0
20	HNO3	1.00E-09	2.00e+05	-8707.	1.87	0.0
21	ISOP	1.00E-09	1.00e-02	0.	1.94	0.0
22	MEOH	1.00E-09	2.20e+02	-4932.	1.33	0.0
23	ETOH	1.00E-09	2.20e+02	-4932.	1.60	0.0
24	ISPD	1.00E-09	6.30e+03	-6492.	1.97	0.0
25	NTR	1.00E-09	9.40e+03	-8706.	2.72	0.0

Reaction Records

	rate const	act energy
1	0.0000E+00	0.0000E+00
2	2.5940E+08	-1.1750E+03
3	1.5984E+03	1.3700E+03
4	8.2500E+05	0.0000E+00
5	1.3854E+05	-6.8700E+02
6	1.4628E+05	-6.0200E+02
7	2.8386E+00	2.4500E+03
8	0.0000E+00	0.0000E+00
9	0.0000E+00	0.0000E+00
10	2.5500E+12	-3.9000E+02

Figure 3-2. Example CAMx chemistry parameters file.

11	1.9560E+07	0.0000E+00
12	6.0000E+03	9.4000E+02
13	1.7994E+02	5.8000E+02
14	0.0000E+00	0.0000E+00
15	2.6500E+06	-2.5000E+02
16	3.5406E+01	1.2300E+03
17	1.1118E+05	-2.5600E+02
18	1.1400E-04	0.0000E+00
19	1.6656E+02	1.0897E+04
20	9.2340E-03	-5.3000E+02
21	9.6000E-10	0.0000E+00
22	5.8794E+05	-8.0600E+02
23	0.0000E+00	0.0000E+00
24	5.8620E+05	0.0000E+00
25	9.0000E-04	0.0000E+00
26	1.0090E+06	-7.1300E+02
27	1.3074E+04	-1.0000E+03
28	7.3620E+05	-2.4000E+02
29	0.0000E+00	0.0000E+00
30	0.0000E+00	0.0000E+00
31	0.0000E+00	0.0000E+00
32	2.4864E+05	-1.1500E+03
33	1.3086E+01	-5.8000E+03
34	0.0000E+00	0.0000E+00
35	1.5120E+05	1.8700E+02
36	1.9320E+04	0.0000E+00
37	9.0000E+05	0.0000E+00
38	0.0000E+00	0.0000E+00
39	0.0000E+00	0.0000E+00
40	1.4220E+04	1.5500E+03
41	5.5800E+01	0.0000E+00
42	3.8160E+04	9.8600E+02
43	1.4400E+06	-2.5000E+02
44	2.2200E+02	0.0000E+00
45	0.0000E+00	0.0000E+00
46	1.6920E+06	1.8000E+02
47	8.2200E+05	-3.8000E+02
48	1.5240E+00	1.3500E+04
49	2.2200E+05	0.0000E+00
50	5.7600E+05	0.0000E+00
51	1.2600E+03	1.7100E+03
52	7.2180E+04	0.0000E+00
53	8.2260E+06	8.0000E+03
54	5.7270E+06	0.0000E+00
55	1.3200E+06	0.0000E+00
56	3.5520E+05	3.2400E+02
57	2.5200E+06	-5.0400E+02
58	1.0800E+00	2.1050E+03
59	6.8100E+02	0.0000E+00
60	6.4800E+04	7.9200E+02
61	7.1520E+05	-4.1100E+02
62	1.6200E-01	2.6330E+03

Figure 3-2. Continued. Example CAMx chemistry parameters file.

63	5.4900E+05	-3.2200E+02
64	7.2000E+05	0.0000E+00
65	1.5000E+04	0.0000E+00
66	3.6600E+06	0.0000E+00
67	1.9500E+06	0.0000E+00
68	1.2000E+06	0.0000E+00
69	0.0000E+00	0.0000E+00
70	2.6400E+06	0.0000E+00
71	9.0000E-01	5.0000E+02
72	2.1720E+06	-1.1600E+02
73	1.5600E+06	0.0000E+00
74	0.0000E+00	0.0000E+00
75	3.1920E+06	0.0000E+00
76	8.8560E+06	0.0000E+00
77	1.1400E+00	0.0000E+00
78	5.9760E+04	0.0000E+00
79	7.2000E+05	0.0000E+00
80	1.2000E+05	-1.3000E+03
81	7.2000E+05	0.0000E+00
82	6.6600E+04	-1.6000E+02
83	4.9000E-03	0.0000E+00
84	9.6000E+04	0.0000E+00
85	2.5800E+05	-1.7600E+02
86	5.3400E+05	-1.3000E+03
87	5.3400E+05	-1.3000E+03
88	1.2000E+05	-1.3000E+03
89	2.4000E+05	-1.3000E+03
90	9.7560E+06	-2.5000E+02
91	1.6667E-02	0.0000E+00
92	2.9800E+06	0.0000E+00
93	6.3000E-01	0.0000E+00
94	8.8680E+01	0.0000E+00
95	0.0000E+00	0.0000E+00
96	1.3200E-02	0.0000E+00

Figure 3-2. Concluded. Example CAMx chemistry parameters file.

```

c-----CAMx v1.10
c
c   CAMx.PRM defines model parameters
c
c   Copyright 1996, ENVIRON International Corporation
c
c   Modifications:
c       none
c
c   NOTE: set MX1D equal to max of MXCOL,MXROW,MXLAY
c
c   parameter (mxcol=137,mxrow=110,mxlay=8,mxspec=25,mxgrid=2)
c   parameter (mx1d=137)
c   parameter (mxradcl=12)
c
c   parameter (mxchdrn=2)
c   parameter (mxnode2=mxcol*mxrow)
c   parameter (mxnode3=mxcol*mxrow*mxlay)
c   parameter (mxnode4=mxcol*mxrow*mxlay*mxspec)
c   parameter (mxrxn=99)
c   parameter (ntempr=91,templo=250.0,temphi=340.0)
c   parameter (mxpht1=6,mxpht2=10)
c   parameter (nozn=5,nalb=5,nhaze=3,nhght=11,nzen=10)
c   parameter (nlu=11)
c   parameter (mxptsrc=19000)
c   parameter (mxpig=25000)

```

Figure 3-3. An example “camx.prm” file used to define important model parameters.

4. REFERENCES

- Carter, W.P. 1996. Condensed Atmospheric Photooxidation Mechanisms for Isoprene. *Atmospheric Environment* Vol. 30, No. 24 pp.4275-4290. 1996.
- Carter, W.P. 1990. A Detailed Mechanism for the Gas-Phase Atmospheric Reactions of Organic Compounds. *Atmospheric Environment* Vol. 24A, 481-518.
- Chock, D.P., 1991. A Comparison of Numerical Methods for Solving the Advection Equation -- III. *Atmos. Environ.*, 25A, 853-871.
- EPA, 1995. A User's guide for the CALPUFF Dispersion Model. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, NC, EPA-454/B-95-006.
- Gery, et. al.. 1989. A photochemical kinetics mechanism for urban and regional scale computer modeling. *J. Geophys. Res.*, 94:12, 925-956.
- Gillani, N. V. and J. E. Pleim, 1996. Sub-grid-scale Features of Anthropogenic Emissions of NO_x and VOC in the Context of Regional Eulerian Models. *Atmos. Environ.*, **30**, 2043-2059.
- Guthrie P.D., G. Yarwood, S.B. Shepard and M.P. Ligocki, 1995. Fast UAM: An Example of an Adaptive Approximation Solver for Atmospheric Chemistry Problems. Presented at SciCADE95, Stanford University, March 28 - April 1, 1995.
- Kumar, N., F.W. Lurmann, A.S. Wexler, S. Pandis, and J.H. Seinfeld, 1996. Development and Application of a Three Dimensional Aerosol Model. Presented at the A&WMA Specialty Conference on Computing in Environmental Resource Management, Research Triangle Park, NC, December 2-4, 1996.
- Kumar, N. and A. G. Russell, 1996. Development of a computationally efficient, reactive sub-grid-scale plume model and the impact in the northeastern United States using increasing levels of chemical detail. *J. Of Geophys. Res.*, **101**, 16,737-16,744.
- Lambert, J. D., 1973. "Computational Methods in Ordinary Differential Equations." John Wiley and Sons Ltd. New York.
- Louis, J.F., 1979. A Parametric Model of Vertical Eddy Fluxes in the Atmosphere. *Bound. Lay. Meteor.* 17, 187-202.
- Maul, P.R., 1980. Atmospheric transport of sulfur compound pollutants. Central Electricity Generating Board, MID/SSD/80/0026/R, Nottingham, England.
- Morris R.E., T.C. Myers, and M.A. Yocke. 1993. Design of the UAM-V Integrated

- Photochemical Modeling System -- Discussion of Model Components and Adaptation of the System to the Lake Michigan, Gulf Coast, and Northeast U.S. Regions. Presented at Regional Photochemical Measurements and Modeling Studies, San Diego, CA, November, 1993.
- Sillman, S., 1995. The use of NO_y , H_2O_2 , and HNO_3 as indicators for ozone - NO_x -hydrocarbon sensitivity in urban locations. *J. of Geophys. Res.*, 100, 14,175-14,188.
- Smagorinsky, J. 1963. General Circulation Experiments with the Primitive Equations: I. The Basic Experiment. *Mon. Wea. Rev.*, 91, 99-164.
- Smolarkiewicz, P.K., 1983. A Simple Positive Definite Advection Scheme with Small Implicit Diffusion. *Mon. Wea. Rev.*, 111, 479-486.
- Wesley, M.L., 1989. Parameterization of Surface Resistances to Gaseous Dry Deposition in Regional-Scale Numerical Models. *Atmos. Environ.*, 23, 1293-1304.
- Whitten, G., H.P. Deuel, C.S. Burton, and J.L. Haney. 1996. Memorandum to OTAG Participants "Overview of the Implementation of an Updated Isoprene Chemistry Mechanism in CB4/UAM-V." (Revised Memorandum, July 22).
- Yarwood, G., R.E. Morris, M.A. Yocke, H. Hobo and T. Chico, 1996a. Development of a Methodology for Source Apportionment of Ozone Concentration Estimates from a Photochemical Grid Model. Presented at the 89th AWMA Annual Meeting, Nashville TN, June 23-28.
- Yarwood, G., G. Wilson, R.E. Morris, and M.A. Yocke. 1996b. User's Guide to the Ozone Tool: Ozone Source Apportionment Technology for UAM-IV.