Chapter 13

THE INITIAL CONCENTRATION AND BOUNDARY CONDITION PROCESSORS

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ABSTRACT

This chapter describes the two processors in the Community Multiscale Air Quality (CMAQ) modeling system that generate the initial concentrations and boundary conditions that are required by the CMAQ Chemical Transport Model (CCTM). The major emphasis is on the functionality incorporated in those processors – the initial condition (ICON) and boundary condition (BCON) processors. The chapter describes how each processor can be used to generate initial concentrations and boundary conditions from one of two sources – from predefined default vertical profiles or from other CMAQ simulation results when model nesting is being performed. A description of generating initial and boundary concentrations for special tracer species is also included. The procedures that are used in both processors for interpolating in both the horizontal and vertical directions are described. A description of methods for converting initial and boundary concentrations from one chemical mechanism form to another is also presented. Finally, the manner in which each processor is applied within the Models-3/CMAQ framework is addressed.

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13.0 THE INITIAL CONCENTRATION AND BOUNDARY CONDITION PROCESSORS

13.1 Introduction

The solution of partial and ordinary differential equations that arise in air quality models requires both initial concentrations (ICs) and boundary conditions (BCs). This chapter describes the Community Multiscale Air Quality (CMAQ) modeling system processors that generate these quantities. In the discussions that follow, they will be referred to as the ICON and BCON processors, respectively. The ICs and BCs generated by these two processors are used by the CMAQ Chemical Transport Model (hereafter referred to as the CCTM). For ICs, the CCTM requires that the concentrations of all model species within each grid cell in the modeling domain be specified for the start of the simulation. Concentrations of all model species at the boundaries of the modeling domain throughout the simulation are required as BCs to the CCTM. The emphasis in this chapter is on how the ICs and BCs are generated rather than on how they are used in the CCTM. The reader is referred to Chapter 5 for a discussion of the latter.

The ICON and BCON processors have been designed to process data as automatically as possible. Users should be aware of certain operational assumptions that are employed by the two processors and the CCTM to insure that their applications are performed in the intended manner, however. The discussion below begins with a brief overview of the processors and their relationship to the CCTM. Several topics that address the various aspects of the IC/BC processing are then presented, including the input sources, spatial interpolation, species processing, and mechanism conversions. The last section provides a brief overview of how the ICON and BCON processors are applied.

13.2 Overview of the ICON and BCON Processors

The ICON and BCON processors generate ICs and BCs for individual model species, which include gas-phase mechanism species, aerosols, nonreactive species and tracer species. The techniques for selecting and processing species data will be discussed in more detail below. It is important to emphasize at the outset, however, that it is not necessary for the ICON and BCON processors to generate ICs and BCs for every species that is being modeled. The CCTM will attempt to extract ICs and BCs for each species being modeled from the input files. If a species is not found on the file, the CCTM will automatically set its ICs and BCs to a minimum threshold limit (i.e., a nominal zero). Any data on an IC or BC file for a species that is not being modeled will simply be ignored by the CCTM. Therefore, the user is encouraged to check the ICON, BCON, and CCTM output logs to insure that the ICs and BCs are being set in the intended manner.

The ICON processor generates species concentrations for every cell in the modeling domain, whereas the BCON processor generates species concentrations for the cells immediately surrounding the modeling domain. At present, the thickness of the boundary cells is limited to one, which is the thickness required for all the transport algorithms currently included as part of

the CCTM (e.g., see Chapter 7). The reader is referred to Chapters 6 and 7 for a description of the CMAQ conventions used in establishing modeling domains and their boundary cells.

Both the ICON and BCON processors write the output ICs and BCs to standard Models-3 Input/Output Application Programmer Interface (I/O API) files: 3-dimensional gridded files for the ICs and 3-dimensional boundary files for the BCs. The opening, formatting, and writing of these files are handled automatically by the ICON and BCON processors. It should be noted, however, that the IO/API has a limit of 120 output variables (i.e., number of species) for any one IO/API file. If the number of output variables exceeds the IO/API maximum, the ICON and BCON processors will generate up to two additional files to hold the outputs. If more than 360 output variables are needed, however, code modifications will need to be made to the ICON and BCON processors and the CCTM to accommodate the additional variables.

13.3   Input Sources

The ICON and BCON processors generate IC and BC files from one of three input sources. The first is a time invariant set of vertical concentration profiles. The second source of input data consists of existing Models-3 IO/API 3-dimensional concentration files, normally generated by the CCTM. The final source of IC and BC data involves the generation of special tracer species concentrations used to test numerical transport algorithms. Each of these will be discussed below. It should be added, however, that the ICON/BCON processors can be bypassed if the user desires to use a different method. The only requirement is that the IC and BC files that are eventually fed to the CCTM must be standard Models-3 IO/API gridded concentration and boundary concentration files. The reader is referred to IO/API documentation for a description of the structure and format of those files (EPA, 1998).

13.3.1 Time Invariant Concentration Profiles

This section describes the manner in which the ICON and BCON processors generate ICs and BCs from predefined, vertical concentration profiles. The CMAQ system contains a set of predefined profiles that can be used to generate the requisite ICs and BCs. These profiles give species concentrations as a function of height, and are spatially independent for the ICON processor and only minimally spatially dependent for the BCON processor. Both the ICON and BCON profile data are time independent. Since these data are not highly resolved, they are typically used when no other information about ICs and BCs is available. It should also be noted that the predefined profile files can be replaced by user developed profile data provided that the replacement files are in the same format as the predefined files. The discussion below begins with a description of the predefined profile data, and is followed by a description of how the user can prepare replacement data.

The default IC and BC profiles have been developed for the RADM2 chemical mechanism and the terrain following sigma-p coordinate system (see Chapter 6 for a discussion of CMAQ coordinate types). Both the IC and BC profiles are intended to represent relatively clean air conditions in the eastern-half of the United States, and have been formulated from available

measurements and results obtained from modeling studies. Thus, they do not represent any specific time period. Although profiles for other chemical mechanisms and vertical coordinate systems are not currently available in the CMAQ system, it may still be possible to use the predefined profiles for these cases. Special procedures are included with the ICON and BCON processors to allow conversion from one vertical resolution and/or chemical mechanism to another. These procedures will be described in sections 13.4.2 and 13.6, respectively.

The predefined profile data are stored in ASCII files in the CMAQ system. Table 13-1 contains a listing of the CMAQ predefined IC profile file. Note that line numbers have been added to the listing for reference. The first three lines contain informational text that is not used by the ICON processor. Line 4 contains the number of vertical layers and the number of species for which profiles have been developed, followed by the vertical coordinate values of the sigma-p levels. The fifth line is blank and is ignored by the ICON processor. Lines 6 through 46 contain vertical profiles for 43 different RADM2 gas-phase species. The species name is given in the first column, followed by mixing ratios (in ppm) for each layer. The first entry for a species corresponds to the lowest layer, whereas the last entry corresponds to the uppermost layer. Lines 47 through 52 contain analogous information for key aerosol species. The units for ASO4I, ASO4J, and ASOIL are $\mu g/m^3$, and the units for NUMATKN, NUMACC, and NUMCOR are number/m^3.

Table 13-2 contains a listing of the corresponding predefined BC profile file. The format for this file is similar to that for the IC file, except that one set of profiles is input for each of the four different boundaries of the modeling domain (i.e., north, east, south and west). The BCON processor uses the appropriate set of profiles to generate the BCs at each edge of the modeling domain. Again, line five is blank and is ignored by the BCON processor.

As indicated above, the user can replace a CMAQ predefined profile file with one of their own provided the same file format is used. As noted in the discussion above, none of the first three text lines nor the fifth line in either file is used. Thus, those lines can contain any information or be blank, but they must be present in the file. The remaining data lines are read in FORTRAN list-directed format, so it is not necessary to align the data by columns. The only formatting requirement is that all inputs be separated by commas or by one or more blanks. The species names must not exceed 16 characters and must not contain any blanks. Also, it is not necessary that a six-layer vertical resolution be used, but at least one layer must be present and no more than 30 are allowed. Note that the number of layer heights on line 4 must be one greater than the actual number of layers used. These layer heights must correspond to the heights of the layer interfaces (i.e., not the mid-layer heights), and the first entry for any profile must be for the lowest level (i.e., ground-level). The input mixing ratios, however, are interpreted as layer average values as opposed to values at the layer interfaces. Finally, note that the BC vertical profile data for each edge begins with a line that contains the edge name. Although the processors do not require that these names be specified explicitly, a line corresponding to the edge name line must be included and the processors expect the data for each edge to be input in the order shown in Table 13-2 (i.e., north, east, south, and west).

13.3.2 CCTM Concentration files

Both the ICON and BCON processors can be configured to generate ICs and BCs from existing Models-3 IO/API 3-dimensional, gridded, concentration files. This situation typically arises when performing a nested model simulation and modeling results are available for a coarser grid. Unlike the predefined profile files described above, the CCTM concentration files are both temporally and spatially resolved, necessitating some additional processing procedures. (The subject of spatial interpolation is described in section 13.4.) It should be added, however, that it is not necessary to use the ICON processor for a model continuation run (i.e., a run in which a model simulation is started at the exact same time that a previous one ended and the same modeling domain is being used). In such cases the CMAQ IO/API concentration file from the previous run may be used directly as the input IC file to the CCTM. However, it will still be necessary to generate a BC input file.

Since ICs are required only for the start of a model simulation, the ICON processor will generate ICs for only one time step. BCs are required throughout a simulation, however, so the user must prescribe the period of record for which to produce outputs. One set of BCs will be generated at each time step for that period of record. To illustrate, consider the case in which a model simulation has been performed for a coarse grid for a 24-hour period of record using 1-hour time steps (i.e., the model concentrations were predicted at hourly intervals). The IO/API gridded concentration file for the coarse grid will then contain species concentrations for 25 time steps, one for the start of the simulation (i.e., the ICs for that simulation) and 24 time steps corresponding to the model predictions at each hour. Now assume that it is desired to generate ICs and BCs for a nested model simulation for the same time period. The user would select the first time step for the ICON output, and the ICON processor would generate ICs for that time step only. For the BCON processor, the period of record for the output BCs would be obtained by selecting the same starting time and setting the duration for outputs at 24 hours. This selection would produce 25 time steps on the output file, one for the start and 24 for each of the subsequent simulation hours. The manner in which the time controls are set is described in the Models-3 User Manual (EPA, 1998).

13.3.3 Tracer Species

The ICON and BCON processors also contain the capability to generate ICs and BCs for special tracer species that can be used to investigate the accuracy of the various transport and diffusion algorithms available in the CCTM system. This capability has been included primarily to facilitate the evaluation of alternative algorithms, and thus would not likely be used in most air quality modeling applications.

ICs and BCs can be generated for eight different tracers. Each one can be used to examine different properties of transport algorithms, and thus can be selected individually for output. They are chosen by including specially defined tracer names in the list of model species. The defined names and a brief description of each tracer species follow. (Note that the ICs for these tracers can be viewed with one of the visualization tools to examine the patterns more closely.)

- IC1_BC0: All ICs in the modeling domain are set to 1.0 and all BCs are set to 0.0.

- IC1_BC1: All ICs in the modeling domain are set to 1.0 and all BCs are set to 1.0.

- IC0_BC1: All ICs in the modeling domain are set to 0.0 and all BCs are set to 1.0.

- STREET: Within any horizontal cross-section of cells, IC cell concentrations are set to either 1.0 or 0.0 such that the overall domain pattern resembles a street grid. All BCs are set to zero.

- CHKBRD: Within any horizontal cross-section of cells, IC cell concentrations are set to either 1.0 or 0.0 such that the overall domain pattern resembles a checkerboard. All BCs are set to zero.

- SPOS_A: ICs and BCs are set such that a concentration mound is centered at cell (10,10) in the modeling domain, and the concentration profile is defined below.

- SPOS_B: ICs and BCs are set such that a concentration mound is centered at cell (10,10) in the modeling domain, and the concentration profile is defined below.

- SPOS_C: ICs and BCs are set such that a concentration mound is centered at cell (10,10) in the modeling domain, and the concentration profile is defined below.

$$h_s = \frac{a^2}{a^2 + (x-x_r)^2 + (y-y_r)^2} \tag{13-1}$$

The last three tracer species are designed for superposition tests of transport algorithms. The base shape of the concentration mounds is described by the Witch of Agnesi surface:where a is the radius of the mound, x_r and y_r define the position of the peak of the mound, and h_s is the height of the mound. In the ICON and BCON processors, a is set to 3 and (x_r, y_r) to (10,10). The three tracer signals h_A, h_B, and h_C for SPOS_A, SPOS_B, and SPOS_C are then defined as follows:

$$h_A = q_{max} (1 + h_s) + q_{min} , \tag{13-2a}$$

$$h_B = 2 q_{max} (1 + h_s) - q_{min} , \tag{13-2b}$$

$$h_C = - q_{max} (1 + h_s) + 2 q_{min} , \tag{13-2c}$$

where q_{max} and q_{min} determine the amplitude and background values of the signals, and both are set to 50 in the ICON and BCON processor. With these signals, the addition of mounds B and C

will yield mound A. Thus, the degree to which h_A - (h_B+ h_C) differs from zero in an advection test provides a measure of the nonlinearity of the advection algorithm.

13.4   Spatial Interpolation

Both the ICON and BCON processors are designed to account for differences in spatial resolution between the input files and the IC/BC output files on an automatic basis.   As described in Chapter 6, the CMAQ system is designed to handle different types of horizontal and vertical coordinate systems. All of the data required to completely specify the horizontal and vertical grid structure are contained in three INCLUDE files that are generated by the Models-3 framework: COORD.EXT, HGRD.EXT, and VGRD.EXT. When the CCTM is compiled (or built), these three files are included with the source code, thereby providing the CCTM with all of the necessary information on the grid structure that is being used. Both the ICON and BCON processors operate in a similar fashion, and thus both processors must be built with the same three INCLUDE files that are used to build the CCTM that will eventually use the ICs and BCs. Grid information on the IC/BC inputs is extracted from the input files themselves, so no additional information is required for them. Note that either the horizontal and vertical coordinates for the input file may be of a different type than that for the output file, or they may be of the same type but have different extents or resolutions.

13.4.1 Horizontal Interpolation

Horizontal interpolation is required when a CCTM concentration file is being used as input to either ICON or BCON and the horizontal coordinate system of the input file differs from that needed for the output file. Such cases typically arise when ICs and BCs are being generated for a nested modeling domain that has a finer resolution than a coarser, outer domain. Note that no horizontal interpolation is necessary if both the input and output domains have the same structure or if the time invariant profiles are being used to generate the ICs and BCs.

Disparities in horizontal grid structure are handled by mapping each vertical column of output cells to a corresponding column of input cells. The vertical concentration profiles corresponding to the input column of cells are then used as the vertical profiles for the output column of cells. Note that some vertical interpolation may also be required as described in the next section. The horizontal mapping is done on the basis of cell proximity. The ground-level latitudes and longitudes at the center of each vertical column of cells are first calculated for both the input and output domains. These computed values are then used to find which input column is closest to each output column. Since the ICON and BCON can compute latitude and longitude for any of the available CMAQ map projections, the horizontal grid coordinate of the input and output files do not have to be the same type.

13.4.2 Vertical Interpolation

In some applications, the ICON and BCON may be required to generate ICs and BCs for a vertical grid system that is different from the one used for the input file. The CCTM is capable of

handling several different vertical grid structures (e.g., sigma-p, sigma-z, pressure, etc.), and each of those grid types can have different vertical resolutions (i.e., different numbers of vertical layers or different spacings with the same number of layers). If the vertical structure of the input and output grids is identical (i.e., both are of the same type and have the same vertical resolution), then the processing of input data to output data is routine because of the one-to-one correspondence of the vertical layers. If the vertical grid types or resolutions are different, however, the ICON and BCON will convert from the input to the output vertical structure in most cases. Conversions from one resolution to another can be performed using either profile data or CCTM concentration files, but conversions from one grid type to another can only be performed when using CCTM concentration files. Both the ICON and BCON processors assume that the vertical grid-type of the profile data is the same as the required output structure, and thus no conversions can be performed in that case. The two different vertical interpolation cases that can be performed by the ICON and BCON processors are described next.

Identical Vertical Grid Types, Different Resolutions. When the input and output vertical grid types are the same but vertical resolutions are different, both ICON and BCON will derive ICs or BCs by linear interpolation using the layer heights contained in the input files and those contained in the COORD.EXT INCLUDE file. These heights are in the units of the vertical coordinate system (e.g., sigma-p, sigma-z, pressure, etc.) rather than height above ground level as measured in distance units such as feet or meters. The vertical resolution of the input IC/BC data can be either greater than or less than the output resolution. Linear interpolation is performed using layer heights that correspond to the middle of the layers. Output concentrations are not always interpolated for the bottommost and topmost layers, however. Output concentrations for all layers with mid-layer heights less than the bottommost mid-layer height in the input file will be set equal to the concentration of that bottommost layer. Similarly, output concentrations for all layers above the input topmost mid-layer height will be set equal to the concentration of the topmost layer.

Different Vertical Grid Types. A complete switch of vertical coordinate types can be carried out when the following two conditions are met: 1) the input IC/BC data are in standard Models-3 IO/API files and 2) the gridded 3-dimensional meteorological files that contain the mid-layer heights for both vertical coordinate systems are also available (see Chapter 12 for a description of these meteorological files). When these conditions are met, the ICON and BCON processors will use linear interpolation to convert from one coordinate system to another. The interpolation is performed in exactly the same manner as described in the previous paragraph, except that the mid-layer heights are taken from the 3-dimensional meteorological files which give the mid-layer heights in meters above ground level for both the input IC/BC data and the output IO/API files. Thus, the meteorological data files containing the layer heights in meters above ground level must be available for *both the input and output grids* before the ICON and BCON processors can be used.

13.5   ICON/BCON Species Processing

The selection of species that are to be modeled and thus require ICs and BCs is controlled by the Program Control Processor (PCP). A detailed description of that processor is contained in Chapter 15, and will not be repeated here. A brief overview of some of the relationships between the PCP and the ICON/BCON processors is presented here to facilitate the description of species processing, however.

The species that are to be modeled in a CCTM simulation are determined when the user invokes the PCP in the Models-3 framework to select a gas phase chemical mechanism, whether or not aerosols are to be included, and whether to include other nonreactive and/or tracer species. The Models-3 framework generates four INCLUDE files that contain the names of all species that are to be modeled -- GC_SPC.EXT, AE_SPC.EXT, NR_SPC.EXT, and TR_SPC.EXT (collectively referred to below as the SPC INCLUDE files). The Models-3 framework also allows the user to invoke special treatment of the ICs and BCs for individual species by defining special surrogate names and providing corresponding scale factors for the calculation of ICs (EPA, 1998). The Models-3 framework generates four INCLUDE files that contain this information -- GC_ICBC.EXT, AE_ICBC.EXT, NR_ICBC.EXT, and TR_ICBC.EXT (collectively referred to below as the ICBC INCLUDE files). Note that some of these files may not contain any entries depending on the user's selection, but all files will be generated by the framework. Just as both the SPC and ICBC INCLUDE files must be included when the CCTM is built, they must also be included when the ICON and BCON processors are built.

The SPC INCLUDE files contain the names of all species to be modeled and will therefore require ICs and BCs in the CCTM. The ICON/BCON processors use the information in both the SPC and the ICBC INCLUDE files to determine which species data should be extracted from the input file and be subsequently written to the output file. The ICON and BCON processors also include an option to convert from one chemical mechanism to another. Since it represents a special option with its own unique rules, it is described separately in section 13.6. The subsequent discussion focuses on the treatment of individual species for two cases - one with and one without associated surrogate names.

Consider first the case in which a surrogate name is not specified. This situation occurs when a model species (i.e., one whose name is included in one of the SPC INCLUDE files) does not have a surrogate name assigned to it. In this case, the ICON and BCON processors simply check to see if the input file contains data for a species with the exact same name as the model species name. If none is found, ICs and BCs are not generated for that species. If a match is found, the data for that species are extracted from the input file, processed, and written to the IC and BC output files.

The assignment of a surrogate name to a particular species complicates the processing slightly. Surrogate names in the CMAQ system arise at least in part from the generalized treatment of the chemical mechanisms and the fact that species names are not "hardwired" in the CMAQ system.

Their primary function is to link a model species with data that are associated with a species of a different name. Two examples are presented to illustrate potential uses.

The first example illustrates how surrogates can be used to provide simple links from one species to another. First, suppose a series of CMAQ model simulations had been performed using the CMAQ system standard RADM2 mechanism in which formaldehyde is named HCHO. Thus, all of the data for that species will be associated with the name HCHO in the CMAQ system data files. Now consider that a researcher wants to make use of that data but will be using their own version of the RADM2 mechanism in which formaldehyde is named FORM. To use the older modeling data, the researcher could either change the formaldehyde name in the chemical mechanism to conform to the original RADM2 name or assign the surrogate HCHO for FORM. In the latter case, both the ICON/BCON processors and the CCTM are designed to extract IC/BC data using the surrogate name in place the model species name. This will be explained in more detail further below.

The second example of using a surrogate name illustrates how scale factors can be used with surrogates. Suppose a researcher is experimenting with a new chemical mechanism which divides a particular species PAR into two new species, PAR1 and PAR2. Further, suppose the researcher wants to use existing CMAQ model simulations with the PAR species to generate ICs and BCs for both PAR1 and PAR2. The researcher will assume that 25% of the PAR IC/BC concentrations will be assigned to PAR1 and 75% to PAR2. To effect this in the CMAQ modeling system, the researcher can assign the species surrogate name PAR to *both* PAR1 and PAR2, and assign 0.25 to the ICBC scale factor for PAR1 species and 0.75 to the ICBC scale factor for PAR2. The ICON/BCON processors and CCTM will use this information to compute the proper ICs and BCs for the two species PAR1 and PAR2 from the input PAR values. The procedures followed by both the ICON/BCON and the CCTM are described next.

The introduction of surrogate names for IC and BC species affects the manner in which both the ICON/BCON processors and the CCTM operate. Consider first the processing that takes place in the ICON/BCON processors. Each species in the SPC INCLUDE files is selected for processing individually. If a surrogate name is assigned to that species, the IC/BC input files are examined to see if the surrogate name is included with the inputs. If the surrogate name is on the input file, the data corresponding to that name are extracted from the input file, processed and output *under the surrogate name*. Further, the ICBC scale factors are not applied in the ICON and BCON. If the surrogate name is not found on the input data file, the ICON/BCON processors will then check the input file using the model species name as if no surrogate name had existed. Again, if a match is found using the model species name, the corresponding data are extracted and output *under the model species name*. If the input file does not contain any data under the surrogate name or the model species name, then no IC/BC data are generated for that particular model species.

Now consider processing in the CCTM when surrogate names are used for ICs/BCs. The CCTM processes each species in the SPC INCLUDE files individually. If a surrogate name is specified for the model species and it is found on the IC/BC input files, the CCTM extracts the data for

that name, applies the scale factor to those data, and then assigns the scaled concentrations to the ICs and BC concentrations for the model species. If the surrogate species name is not found on the input IC/BC files, the input file is checked using the model species name contained in the SPC INCLUDE files. If data for that model species are found, then the data are extracted and used directly as ICs and BCs (i.e., no scale factors are applied). If data for the species are not found on the input file, the ICs and BCs are set to the lower threshold limits.

For most routine applications, users need not concern themselves with surrogate mapping issues. The ICON and BCON processors are designed to generate the appropriate ICs and BCs with minimal user interaction, *provided the correct input files and include files are used with the processors.* Both the ICON and the BCON processors generate a species map on the output log that reports the relationship between the input and output IC and BC species. The user can check these logs to insure that the desired species mapping has been performed. Further, the CCTM's output log lists those species for which the lower threshold limits are used, and these should be checked to insure that the ICs/BCs for an important species have not been omitted.

13.6   Mechanism Conversions

The vertical profile data and the CCTM concentration file data that were described above normally correspond to one gas-phase, chemical mechanism. For example, the predefined, vertical profile data presently in the CMAQ system were developed for the RADM2 chemical mechanism. The capability to convert from one gas phase chemical mechanism to another has been included in the ICON and BCON processors, however. It should be emphasized that there is not always a definite correspondence between chemical mechanism species, and it is usually necessary to make several assumptions to make such conversions. This is particularly true for organic species that may be defined differently in two mechanisms. Nevertheless, some simple mechanism conversion capabilities have been included for those cases in which approximations are acceptable for converting from one mechanism to another.

A special routine to generate ICs and BCs for the CB4 chemical mechanism from RADM2 gas-phase mechanism inputs is included as part of the ICON and BCON processor options. At present, no other "hardwired" conversion routines are available in the system, but it is conceivable that some could be added in the future as more chemical mechanisms are added to the CMAQ system. No conversion from CB4 to RADM2 format has been included because the carbon bond lumping technique makes it difficult to disaggregate mechanism species into their original chemical compounds. For a description of these two mechanisms, the reader is referred to Chapter 8. The hardwired RADM2 to CB4 conversion procedures that are used are the same as for the generalized conversion processor that is described next.

As a convenience for the user, a generalized mechanism conversion processor has also been included in both the ICON and BCON processors. This conversion procedure requires the user to generate an ASCII input file that contains mechanism conversion rules. Thus, the user is responsible for defining how the mechanism conversion is to be performed. An example file showing the conversion from RADM2 to CB4 is included in Table 13-3. The file contains the

expressions that are used to convert the ICs and BCs from one mechanism form to another. The ICs and BCs for the CB4 species (i.e., those on the left hand side of the equal sign) are computed from the RADM2 species concentrations (i.e., those on the right hand side of the equal sign) according to the equations shown. As is evident, there is a simple one-to-one correspondence for most species and lumping only occurs for relatively few species. It should also be noted that no conversions will be performed for those species that are not included in the input file, and thus no ICs or BCs will be generated for them. As mentioned previously, the user is advised to review the species map on the ICON/BCON output log to insure that the conversions are being done as intended. Finally, it should be added that the mechanism conversion option applies only to the gas phase chemistry species. Aerosol, nonreactive and tracer species will be processed in the standard way, regardless of whether a mechanism conversion is being performed.

The format for the mechanism conversion rules is relatively simple. Species names must be 16 characters or less and not contain any blanks. Only one species is permitted on the left-hand side of the equation, and the species name should correspond to a name in the output mechanism. The equal sign must be present, and at least one species name must appear to the right of it. Coefficients for species are allowed on the right-hand side only, and they can be in either integer, real, or exponential format. They must always be followed by an asterisk to indicate multiplication. For expressions involving lumping of species, only addition is allowed and it is indicated by a plus sign. Line-wrap is allowed so that a single lumping rule can span more than one line. Each conversion rule must conclude with a semicolon, and the last command must be "END;". Finally, the input files are read in a free form input that generally ignores white spaces between species names, coefficients, operators and line terminators.

13.7   ICON/BCON Applications

This section provides an overview of how the ICON and BCON processors are applied in practice. Applications are normally carried out in two steps: compilation (or building) and execution. As mentioned earlier, when the ICON and BCON executables are built, the grid INCLUDE files for the modeling domain must be included. In addition, the user must select four modules that determine the ICON/BCON processing routines to incorporate when the executable is built. Two modules must always be present: *icon* (or *bcon* in the case of the BCON processor) and *icl*. These two modules contain processing routines that are common to all applications. One of the following three modules must be chosen to include the routines to process the specific input source: 1) *profile* for using a time invariant vertical concentration profile contained in an ASCII file, 2) *m3conc* for processing a CMAQ IO/API concentration file, or 3) *tracer* for generating special tracer species ICs and BCs. Finally, one of three modules must also be selected to control the mechanism conversion procedure: 1) *noop* for no mechanism conversion, 2) *radm2_to_cb4* for a CMAQ predefined RADM2 to CB4 conversion, or 3) *user_defined* to process a user generated ASCII file (e.g., Table 13-3) containing mechanism conversion rules that are used to generate ICs and BCs for one mechanism using input concentrations for a different mechanism.

The second step involves running the processors with all necessary input files assigned and the time control parameters set. Both are provided to the processors by means of environment variables. The input and output files are assigned by means of predefined logical file names. The ICON processor requires a starting date and time in the Models-3 conventional time stamp format. The BCON processor requires both a starting date and time and a run duration parameter.

For detailed information on compiling and running these processors, the reader is referred to the Models-3 User Manual (EPA, 1998).

13.8   References

EPA, 1998. *Models-3 Volume 9b: User Manual*, Draft EPA report, U. S. Environmental Protection Agency, Research Triangle Park, N.C.

This chapter is taken from *Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System*, **edited by D. W. Byun and J. K. S. Ching, 1999.**

Table 13-1. CMAQ Predefined Vertical Profiles for Initial Concentrations

```
 1 Optional boundary condition: The vertical coordinate of the model to
 2 generate these b.c. is the terrain-following sigma coordinate. The number of
 3 sigma  layers and defined sigma levels are listed below.
 4 6      47   1.00  0.98  0.93  0.84  0.60  0.30  0.00
 5
 6 SO2        0.300E-03  0.200E-03  0.100E-03  0.100E-03  0.200E-04  0.100E-04
 7 SULF       0.150E-03  0.150E-03  0.100E-03  0.100E-03  0.200E-04  0.100E-04
 8 NO2        0.200E-04  0.200E-04  0.100E-04  0.000E+00  0.000E+00  0.000E+00
 9 NO         0.200E-04  0.200E-04  0.100E-04  0.000E+00  0.000E+00  0.000E+00
10 O3         0.350E-01  0.350E-01  0.400E-01  0.500E-01  0.600E-01  0.700E-01
11 HNO3       0.500E-04  0.500E-04  0.500E-04  0.500E-04  0.700E-04  0.100E-03
12 H2O2       0.100E-02  0.100E-02  0.150E-02  0.100E-02  0.800E-03  0.200E-03
13 ALD        0.300E-04  0.350E-04  0.300E-04  0.200E-04  0.200E-04  0.100E-04
14 HCHO       0.250E-03  0.250E-03  0.250E-03  0.200E-03  0.100E-03  0.500E-04
15 OP1        0.250E-06  0.250E-06  0.250E-06  0.200E-06  0.100E-06  0.500E-07
16 OP2        0.300E-07  0.350E-07  0.300E-07  0.200E-07  0.200E-07  0.100E-07
17 PAA        0.300E-04  0.300E-04  0.300E-04  0.250E-04  0.200E-04  0.150E-04
18 ORA1       0.100E-05  0.100E-05  0.500E-06  0.500E-06  0.500E-06  0.000E+00
19 ORA2       0.100E-05  0.100E-05  0.500E-06  0.500E-06  0.500E-06  0.000E+00
20 NH3        0.100E-03  0.100E-03  0.300E-04  0.200E-04  0.200E-04  0.100E-04
21 N2O5       0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
22 NO3        0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
23 PAN        0.200E-04  0.200E-04  0.100E-04  0.100E-04  0.100E-04  0.000E+00
24 HC3        0.400E-04  0.400E-04  0.320E-04  0.120E-04  0.400E-05  0.000E+00
25 HC5        0.400E-04  0.400E-04  0.320E-04  0.120E-04  0.400E-05  0.000E+00
26 HC8        0.200E-04  0.200E-04  0.160E-04  0.600E-05  0.200E-05  0.000E+00
27 ETH        0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
28 CO         0.800E-01  0.800E-01  0.800E-01  0.700E-01  0.650E-01  0.500E-01
29 OL2        0.500E-05  0.300E-05  0.200E-05  0.100E-05  0.100E-05  0.000E+00
30 OLT        0.200E-06  0.200E-06  0.100E-06  0.000E+00  0.000E+00  0.000E+00
31 OLI        0.100E-06  0.100E-06  0.000E+00  0.000E+00  0.000E+00  0.000E+00
32 TOL        0.100E-05  0.100E-05  0.100E-05  0.100E-05  0.000E+00  0.000E+00
33 XYL        0.200E-06  0.200E-06  0.100E-06  0.000E+00  0.000E+00  0.000E+00
34 ACO3       0.100E-08  0.100E-08  0.100E-08  0.100E-08  0.100E-08  0.100E-08
35 TPAN       0.100E-07  0.100E-07  0.100E-07  0.100E-07  0.100E-07  0.100E-07
36 HONO       0.100E-08  0.100E-08  0.100E-08  0.100E-08  0.100E-08  0.100E-08
37 HNO4       0.200E-08  0.200E-08  0.200E-08  0.200E-08  0.200E-08  0.200E-08
38 KET        0.300E-04  0.350E-04  0.300E-04  0.200E-04  0.200E-04  0.100E-04
39 GLY        0.250E-06  0.250E-06  0.250E-06  0.200E-06  0.100E-06  0.500E-07
40 MGLY       0.250E-06  0.250E-06  0.250E-06  0.200E-06  0.100E-06  0.500E-07
41 DCB        0.250E-06  0.250E-06  0.250E-06  0.200E-06  0.100E-06  0.500E-07
42 ONIT       0.200E-04  0.200E-04  0.160E-04  0.600E-05  0.200E-05  0.000E+00
43 CSL        0.100E-08  0.100E-08  0.100E-08  0.100E-08  0.100E-08  0.100E-08
44 ISO        0.250E-05  0.250E-05  0.250E-05  0.250E-05  0.250E-05  0.250E-05
45 HO         0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
46 HO2        0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
47 ASO4I      4.810E-02  3.207E-02  1.603E-02  1.603E-02  3.207E-03  1.603E-03
48 ASO4J      1.154E+00  7.696E-01  3.848E-01  3.848E-01  7.696E-02  3.848E-02
49 NUMATKN    1.437E+10  9.583E+09  4.791E+09  4.791E+09  9.583E+08  4.791E+08
50 NUMACC     4.110E+08  2.740E+08  1.370E+08  1.370E+08  2.740E+07  1.370E+07
51 ASOIL      1.000E+00  8.000E-01  4.000E-01  4.000E-01  8.000E-02  4.000E-02
52 NUMCOR     1.740E+04  1.392E+04  6.960E+03  6.960E+03  1.392E+03  6.960E+02
```

Table 13-2. CMAQ Predefined Vertical Profiles for Boundary Conditions

```
 1  Optional boundary condition: The vertical coordinate of the model to
 2  generate these b.c. is the terrain-following sigma coordinate. The number of
 3  sigma layers and defined sigma levels are listed below.
 4  6      47    1.00   0.98   0.93   0.84   0.60   0.30   0.00
 5
 6   North
 7
 8  SO2        0.300E-03   0.200E-03   0.100E-03   0.100E-03   0.200E-04   0.100E-04
 9  SULF       0.150E-03   0.150E-03   0.100E-03   0.100E-03   0.200E-04   0.100E-04
10  NO2        0.200E-04   0.200E-04   0.100E-04   0.000E+00   0.000E+00   0.000E+00
11  NO         0.200E-04   0.200E-04   0.100E-04   0.000E+00   0.000E+00   0.000E+00
12  O3         0.350E-01   0.350E-01   0.400E-01   0.500E-01   0.600E-01   0.700E-01
13  HNO3       0.500E-04   0.500E-04   0.500E-04   0.500E-04   0.700E-04   0.100E-03
14  H2O2       0.100E-02   0.100E-02   0.150E-02   0.100E-02   0.800E-03   0.200E-03
15  ALD        0.300E-04   0.350E-04   0.300E-04   0.200E-04   0.200E-04   0.100E-04
16  HCHO       0.250E-03   0.250E-03   0.250E-03   0.200E-03   0.100E-03   0.500E-04
17  OP1        0.250E-06   0.250E-06   0.250E-06   0.200E-06   0.100E-06   0.500E-07
18  OP2        0.300E-07   0.350E-07   0.300E-07   0.200E-07   0.200E-07   0.100E-07
19  PAA        0.300E-04   0.300E-04   0.300E-04   0.250E-04   0.200E-04   0.150E-04
20  ORA1       0.100E-05   0.100E-05   0.500E-06   0.500E-06   0.500E-06   0.000E+00
21  ORA2       0.100E-05   0.100E-05   0.500E-06   0.500E-06   0.500E-06   0.000E+00
22  NH3        0.100E-03   0.100E-03   0.300E-04   0.200E-04   0.200E-04   0.100E-04
23  N2O5       0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
24  NO3        0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
25  PAN        0.200E-04   0.200E-04   0.100E-04   0.100E-04   0.100E-04   0.000E+00
26  HC3        0.400E-04   0.400E-04   0.320E-04   0.120E-04   0.400E-05   0.000E+00
27  HC5        0.400E-04   0.400E-04   0.320E-04   0.120E-04   0.400E-05   0.000E+00
28  HC8        0.200E-04   0.200E-04   0.160E-04   0.600E-05   0.200E-05   0.000E+00
29  ETH        0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
30  CO         0.800E-01   0.800E-01   0.800E-01   0.700E-01   0.650E-01   0.500E-01
31  OL2        0.500E-05   0.300E-05   0.200E-05   0.100E-05   0.100E-05   0.000E+00
32  OLT        0.200E-06   0.200E-06   0.100E-06   0.000E+00   0.000E+00   0.000E+00
33  OLI        0.100E-06   0.100E-06   0.000E+00   0.000E+00   0.000E+00   0.000E+00
34  TOL        0.100E-05   0.100E-05   0.100E-05   0.100E-05   0.000E+00   0.000E+00
35  XYL        0.200E-06   0.200E-06   0.100E-06   0.000E+00   0.000E+00   0.000E+00
36  ACO3       0.100E-08   0.100E-08   0.100E-08   0.100E-08   0.100E-08   0.100E-08
37  TPAN       0.100E-07   0.100E-07   0.100E-07   0.100E-07   0.100E-07   0.100E-07
38  HONO       0.100E-08   0.100E-08   0.100E-08   0.100E-08   0.100E-08   0.100E-08
39  HNO4       0.200E-08   0.200E-08   0.200E-08   0.200E-08   0.200E-08   0.200E-08
40  KET        0.300E-04   0.350E-04   0.300E-04   0.200E-04   0.200E-04   0.100E-04
41  GLY        0.250E-06   0.250E-06   0.250E-06   0.200E-06   0.100E-06   0.500E-07
42  MGLY       0.250E-06   0.250E-06   0.250E-06   0.200E-06   0.100E-06   0.500E-07
43  DCB        0.250E-06   0.250E-06   0.250E-06   0.200E-06   0.100E-06   0.500E-07
44  ONIT       0.200E-04   0.200E-04   0.160E-04   0.600E-05   0.200E-05   0.000E+00
45  CSL        0.100E-08   0.100E-08   0.100E-08   0.100E-08   0.100E-08   0.100E-08
46  ISO        0.250E-05   0.250E-05   0.250E-05   0.250E-05   0.250E-05   0.250E-05
47  HO         0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
48  HO2        0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
49  ASO4I      2.405E-02   2.405E-02   1.603E-02   1.603E-02   3.207E-03   1.603E-03
50  ASO4J      5.772E-01   5.772E-01   3.848E-01   3.848E-01   7.696E-02   3.848E-02
51  NUMATKN    7.187E+09   7.187E+09   4.791E+09   4.791E+09   9.583E+08   4.791E+08
52  NUMACC     2.055E+08   2.055E+08   1.370E+08   1.370E+08   2.740E+07   1.370E+07
53  ASOIL      5.000E-01   5.000E-01   4.000E-01   4.000E-01   8.000E-01   3.000E-01
54  NUMCOR     8.750E+03   8.750E+03   7.000E+03   7.000E+03   1.400E+03   5.250E+02
55   East
56
57  SO2        0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
58  SULF       0.200E-03   0.200E-03   0.200E-03   0.200E-03   0.200E-04   0.100E-04
```

Table 13-2. CMAQ Predefined Vertical Profiles for Boundary Conditions

59	NO2	0.100E-04	0.100E-04	0.000E+00	0.000E+00	0.000E+00	0.000E+00
60	NO	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
61	O3	0.300E-01	0.350E-01	0.400E-01	0.500E-01	0.600E-01	0.700E-01
62	HNO3	0.500E-04	0.500E-04	0.500E-04	0.500E-04	0.500E-04	0.150E-03
63	H2O2	0.200E-02	0.200E-02	0.200E-02	0.200E-02	0.150E-02	0.150E-02
64	ALD	0.400E-04	0.400E-04	0.400E-04	0.400E-04	0.400E-04	0.400E-04
65	HCHO	0.250E-03	0.250E-03	0.250E-03	0.200E-03	0.150E-03	0.100E-03
66	OP1	0.250E-06	0.250E-06	0.250E-06	0.200E-06	0.150E-06	0.100E-06
67	OP2	0.400E-07	0.400E-07	0.400E-07	0.400E-07	0.400E-07	0.400E-07
68	PAA	0.500E-04	0.500E-04	0.500E-04	0.500E-04	0.500E-04	0.500E-04
69	ORA1	0.150E-05	0.500E-06	0.500E-06	0.500E-06	0.500E-06	0.500E-06
70	ORA2	0.150E-05	0.500E-06	0.500E-06	0.500E-06	0.500E-06	0.500E-06
71	NH3	0.500E-04	0.500E-04	0.500E-04	0.200E-04	0.200E-04	0.200E-04
72	N2O5	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
73	NO3	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
74	PAN	0.100E-04	0.100E-04	0.100E-04	0.100E-04	0.100E-04	0.100E-04
75	HC3	0.120E-04	0.120E-04	0.120E-04	0.800E-05	0.400E-05	0.400E-05
76	HC5	0.120E-04	0.120E-04	0.120E-04	0.800E-05	0.400E-05	0.400E-05
77	HC8	0.600E-05	0.600E-05	0.600E-05	0.400E-05	0.200E-05	0.200E-05
78	ETH	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
79	CO	0.800E-01	0.800E-01	0.800E-01	0.750E-01	0.700E-01	0.650E-01
80	OL2	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
81	OLT	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
82	OLI	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
83	TOL	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
84	XYL	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
85	ACO3	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08
86	TPAN	0.100E-07	0.100E-07	0.100E-07	0.100E-07	0.100E-07	0.100E-07
87	HONO	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08
88	HNO4	0.200E-08	0.200E-08	0.200E-08	0.200E-08	0.200E-08	0.200E-08
89	KET	0.400E-04	0.400E-04	0.400E-04	0.400E-04	0.400E-04	0.400E-04
90	GLY	0.250E-06	0.250E-06	0.250E-06	0.200E-06	0.150E-06	0.100E-06
91	MGLY	0.250E-06	0.250E-06	0.250E-06	0.200E-06	0.150E-06	0.100E-06
92	DCB	0.250E-06	0.250E-06	0.250E-06	0.200E-06	0.150E-06	0.100E-06
93	ONIT	0.600E-05	0.600E-05	0.600E-05	0.400E-05	0.200E-05	0.200E-05
94	CSL	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08
95	ISO	0.250E-05	0.250E-05	0.250E-05	0.250E-05	0.250E-05	0.250E-05
96	HO	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
97	HO2	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
98	ASO4I	3.207E-02	3.207E-02	3.207E-02	3.207E-02	3.207E-03	1.603E-03
99	ASO4J	7.696E-01	7.696E-01	7.696E-01	7.696E-01	7.696E-02	3.848E-02
100	NUMATKN	9.583E+09	9.583E+09	9.583E+09	9.583E+09	9.583E+08	4.791E+08
101	NUMACC	2.740E+08	2.740E+08	2.740E+08	2.740E+08	2.740E+07	1.370E+07
102	ASOIL	8.000E-01	8.000E-01	8.000E-01	8.000E-01	8.000E-02	4.000E-02
103	NUMCOR	1.392E+04	1.392E+04	1.392E+04	1.392E+04	1.392E+03	6.960E+02
104	South						
105							
106	SO2	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
107	SULF	0.200E-03	0.200E-03	0.200E-03	0.100E-03	0.500E-04	0.200E-04
108	NO2	0.100E-04	0.100E-04	0.000E+00	0.000E+00	0.000E+00	0.000E+00
109	NO	0.100E-04	0.100E-04	0.000E+00	0.000E+00	0.000E+00	0.000E+00
110	O3	0.300E-01	0.350E-01	0.400E-01	0.500E-01	0.600E-01	0.700E-01
111	HNO3	0.500E-04	0.500E-04	0.500E-04	0.500E-04	0.500E-04	0.150E-03
112	H2O2	0.200E-02	0.200E-02	0.200E-02	0.200E-02	0.150E-02	0.100E-02
113	ALD	0.400E-04	0.400E-04	0.400E-04	0.400E-04	0.400E-04	0.500E-05
114	HCHO	0.250E-03	0.250E-03	0.250E-03	0.200E-03	0.150E-03	0.100E-03
115	OP1	0.250E-06	0.250E-06	0.250E-06	0.200E-06	0.150E-06	0.100E-06
116	OP2	0.400E-07	0.400E-07	0.400E-07	0.400E-07	0.400E-07	0.500E-08
117	PAA	0.100E-03	0.100E-03	0.100E-03	0.100E-03	0.500E-04	0.500E-04

Table 13-2. CMAQ Predefined Vertical Profiles for Boundary Conditions

118	ORA1	0.150E-05	0.500E-06	0.500E-06	0.500E-06	0.500E-06	0.500E-06
119	ORA2	0.150E-05	0.500E-06	0.500E-06	0.500E-06	0.500E-06	0.500E-06
120	NH3	0.500E-04	0.500E-04	0.500E-04	0.300E-04	0.200E-04	0.200E-04
121	N2O5	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
122	NO3	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
123	PAN	0.100E-04	0.100E-04	0.100E-04	0.100E-04	0.100E-04	0.100E-04
124	HC3	0.120E-04	0.120E-04	0.120E-04	0.400E-05	0.400E-05	0.400E-05
125	HC5	0.120E-04	0.120E-04	0.120E-04	0.400E-05	0.400E-05	0.400E-05
126	HC8	0.600E-05	0.600E-05	0.600E-05	0.200E-05	0.200E-05	0.200E-05
127	ETH	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
128	CO	0.700E-01	0.700E-01	0.700E-01	0.700E-01	0.650E-01	0.550E-01
129	OL2	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
130	OLT	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
131	OLI	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
132	TOL	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
133	XYL	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
134	ACO3	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08
135	TPAN	0.100E-07	0.100E-07	0.100E-07	0.100E-07	0.100E-07	0.100E-07
136	HONO	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08
137	HNO4	0.200E-08	0.200E-08	0.200E-08	0.200E-08	0.200E-08	0.200E-08
138	KET	0.400E-04	0.400E-04	0.400E-04	0.400E-04	0.400E-04	0.500E-05
139	GLY	0.250E-06	0.250E-06	0.250E-06	0.200E-06	0.150E-06	0.100E-06
140	MGLY	0.250E-06	0.250E-06	0.250E-06	0.200E-06	0.150E-06	0.100E-06
141	DCB	0.250E-06	0.250E-06	0.250E-06	0.200E-06	0.150E-06	0.100E-06
142	ONIT	0.600E-05	0.600E-05	0.600E-05	0.200E-05	0.200E-05	0.200E-05
143	CSL	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08
144	ISO	0.250E-05	0.250E-05	0.250E-05	0.250E-05	0.250E-05	0.250E-05
145	HO	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
146	HO2	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
147	ASO4I	3.207E-02	3.207E-02	3.207E-02	1.603E-02	3.207E-03	1.603E-03
148	ASO4J	7.696E-01	7.696E-01	7.696E-01	3.848E-01	7.696E-02	3.848E-02
149	NUMATKN	9.583E+09	9.583E+09	9.583E+09	4.791E+09	9.583E+08	4.791E+08
150	NUMACC	2.740E+08	2.740E+08	2.740E+08	1.370E+08	2.740E+07	1.370E+07
151	ASOIL	8.000E-01	8.000E-01	8.000E-01	4.000E-01	8.000E-02	4.000E-02
152	NUMCOR	1.400E+04	1.400E+04	1.400E+04	7.000E+03	1.400E+03	7.000E+02
153	West						
154							
155	SO2	0.300E-03	0.200E-03	0.200E-03	0.100E-03	0.000E+00	0.000E+00
156	SULF	0.300E-03	0.200E-03	0.200E-03	0.100E-03	0.000E+00	0.000E+00
157	NO2	0.100E-03	0.100E-03	0.100E-03	0.500E-04	0.000E+00	0.000E+00
158	NO	0.500E-04	0.500E-04	0.500E-04	0.200E-04	0.000E+00	0.000E+00
159	O3	0.350E-01	0.400E-01	0.450E-01	0.500E-01	0.600E-01	0.700E-01
160	HNO3	0.500E-03	0.500E-03	0.500E-03	0.500E-03	0.200E-03	0.100E-03
161	H2O2	0.200E-02	0.200E-02	0.200E-02	0.200E-02	0.800E-03	0.200E-03
162	ALD	0.400E-04	0.400E-04	0.400E-04	0.400E-04	0.400E-04	0.500E-05
163	HCHO	0.400E-03	0.400E-03	0.400E-03	0.400E-03	0.100E-03	0.500E-04
164	OP1	0.400E-06	0.400E-06	0.400E-06	0.400E-06	0.100E-06	0.500E-07
165	OP2	0.400E-07	0.400E-07	0.400E-07	0.400E-07	0.400E-07	0.500E-08
166	PAA	0.250E-04	0.250E-04	0.250E-04	0.250E-04	0.200E-04	0.100E-04
167	ORA1	0.250E-05	0.250E-05	0.250E-05	0.250E-05	0.500E-06	0.500E-06
168	ORA2	0.250E-05	0.250E-05	0.250E-05	0.250E-05	0.500E-06	0.500E-06
169	NH3	0.300E-03	0.300E-03	0.300E-03	0.200E-03	0.100E-03	0.500E-04
170	N2O5	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
171	NO3	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
172	PAN	0.100E-03	0.100E-03	0.100E-03	0.500E-04	0.100E-04	0.100E-04
173	HC3	0.800E-04	0.800E-04	0.800E-04	0.600E-04	0.800E-05	0.400E-05
174	HC5	0.800E-04	0.800E-04	0.800E-04	0.600E-04	0.800E-05	0.400E-05
175	HC8	0.400E-04	0.400E-04	0.400E-04	0.300E-04	0.400E-05	0.200E-05
176	ETH	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

Table 13-2. CMAQ Predefined Vertical Profiles for Boundary Conditions

177	CO	0.800E-01	0.800E-01	0.800E-01	0.800E-01	0.650E-01	0.500E-01
178	OL2	0.100E-04	0.100E-04	0.500E-05	0.500E-05	0.100E-05	0.000E+00
179	OLT	0.200E-05	0.100E-05	0.500E-06	0.300E-06	0.000E+00	0.000E+00
180	OLI	0.100E-05	0.200E-06	0.100E-06	0.000E+00	0.000E+00	0.000E+00
181	TOL	0.100E-04	0.500E-05	0.500E-05	0.300E-05	0.000E+00	0.000E+00
182	XYL	0.300E-05	0.200E-05	0.400E-06	0.400E-06	0.000E+00	0.000E+00
183	ACO3	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08
184	TPAN	0.100E-07	0.100E-07	0.100E-07	0.100E-07	0.100E-07	0.100E-07
185	HONO	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08
186	HNO4	0.200E-08	0.200E-08	0.200E-08	0.200E-08	0.200E-08	0.200E-08
187	KET	0.400E-04	0.400E-04	0.400E-04	0.400E-04	0.400E-04	0.500E-05
188	GLY	0.400E-06	0.400E-06	0.400E-06	0.400E-06	0.100E-06	0.500E-07
189	MGLY	0.400E-06	0.400E-06	0.400E-06	0.400E-06	0.100E-06	0.500E-07
190	DCB	0.400E-06	0.400E-06	0.400E-06	0.400E-06	0.100E-06	0.500E-07
191	ONIT	0.400E-04	0.400E-04	0.400E-04	0.300E-04	0.400E-05	0.200E-05
192	CSL	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08	0.100E-08
193	ISO	0.250E-05	0.250E-05	0.250E-05	0.250E-05	0.250E-05	0.250E-05
194	HO	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
195	HO2	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
196	ASO4I	4.810E-02	3.207E-02	3.207E-02	1.603E-02	3.207E-03	1.603E-03
197	ASO4J	1.154E+00	7.696E-01	7.696E-01	3.848E-01	7.696E-02	3.848E-02
198	NUMATKN	1.437E+10	9.583E+09	9.583E+09	4.791E+09	9.583E+08	4.791E+08
199	NUMACC	4.110E+08	2.740E+08	2.740E+08	1.370E+08	2.740E+07	1.370E+07
200	ASOIL	1.000E+00	8.000E-01	8.000E-01	4.000E-01	8.000E-02	4.000E-02
201	NUMCOR	1.750E+04	1.400E+04	1.400E+04	7.000E+03	1.400E+03	7.000E+02

Table 13-3. Example RADM2 to CB4 Conversion Rules

```
  NO2  =         NO2 ;
   NO   =         NO ;
   O    =         O3P;
   O3   =         O3 ;
   NO3  =         NO3;
   O1D  =         O1D;
   OH   =         HO ;
   HO2  =         HO2 ;
   N2O5 =         N2O5;
   HNO3 =         HNO3;
   HONO =         HONO;
   PNA  =         HNO4;
   H2O2 =         H2O2;
   CO   =         CO;
   SO2  =         SO2;
   SULF =         SULF;
   PAN  =         PAN;
   FACD =         ORA1;
   AACD =         ORA2;
   PACD =         PAA;
   UMHP =         OP1;
   MGLY =         MGLY;
   OPEN =         DCB;
   CRES =         CSL;
   FORM =         HCHO + 1.0 * GLY;
   ALD2 = 1.0 *   ALD  + 2.0 * OLI;
   PAR  = 0.4 *   ETH  + 2.9 * HC3  + 4.8 * HC5  +
          7.9 *   HC8  + 0.8 * OLT  + 0.8 * OLI  +
          3.9 *   KET;
   OLE  =         OLT;
   TOL  =         TOL;
   ISOP =         ISO;
   ETH  =         OL2;
   XYL  =         XYL;
   TERP =         TERP;
  END;
```