USER'S GUIDE
EMISSIONS PROCESSOR

VERSION 3

ENVIRON International Corporation
773 San Marin Drive, Suite 2115
Novato, CA 94998
415-899-0700

www.environcorp.com

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1. INTRODUCTION

Under the 1990 Clean Air Act Amendments, air quality analyses using photochemical grid models are required for areas designated as serious, severe, and extreme ozone nonattainment areas and multistate moderate ozone nonattainment areas. Proposed 2007 revisions to the National Ambient Air Quality Standards (NAAQS) for ozone strengthen the criteria for ground-level ozone. A key component of any photochemical modeling effort is the preparation of a detailed emissions inventory. For purposes of photochemical modeling, an emissions inventory consists of emissions estimates that have been temporally allocated, spatially distributed and chemically speciated. These are the tasks performed by the EPS3 system. This section provides a general discussion of modeling inventory requirements and methodologies.

1.1   CONCEPTUAL OVERVIEW OF A MODELING INVENTORY

Most 3-dimensional photochemical grid models are designed to calculate concentrations of both inert and chemically reactive pollutants by simulating physical and chemical processes which occur in the atmosphere. These calculations are based on the atmospheric diffusivity or chemical mechanism compound continuity equation, which represents a mass balance in which all relevant processes (precursor emissions, transport, diffusion, chemical reactions, and removal processes) are expressed in mathematical terms. For ozone assessment, the model is usually applied for a multi-day period during which adverse meteorological conditions result in elevated concentrations. For carbon monoxide simulations, the model is usually applied for shorter time periods (e.g., 8 to 16 hours). And for particulate simulations, the model is often applied for a modeling period spanning months, often as long as a year.

Major factors affecting photochemical air quality include:

Spatial (vertical and horizontal) and temporal distribution of anthropogenic and biogenic emissions;

Chemical composition of the emitted emissions NO_x, VOC, and $PM_{2.5}$;

Spatial and temporal variations in wind fields;

Dynamics of the boundary layer, including stability and mixing;

Chemical reactions involving VOC, NO_x, CO, and other important compounds;

Diurnal variations of solar radiation and temperature;

Loss of ozone and ozone precursors by dry deposition; and

Ambient background concentrations of VOC, NO_x, CO, and other pollutants within, immediately upwind of, and above the study region.

In a modeling application these processes are simulated for the pollutant of interest (in general, either summertime ozone concentrations or wintertime carbon monoxide concentrations). The model solves the chemical continuity equation for each time step in each grid cell of the

modeling domain; the maximum time step is a function of grid size and the maximum wind velocity. Typical time steps for urban-scale simulations are on the order of 3 to 6 minutes.

Since the model accounts for spatial and temporal variations as well as reactivity differences (i.e., the hydrocarbon composition) of emissions, it is ideally suited for evaluating the effects of emission control scenarios on urban air quality. In practice, a historical ozone (or carbon monoxide) episode is replicated to establish a base case simulation. Model inputs are prepared from observed meteorological, emission, and air quality data for a particular day or days. Once the base case results have been evaluated and determined to perform within prescribed levels, future air quality conditions can be simulated using the meteorological inputs from the base case and a projected emission inventory that reflects future changes in emissions due to population growth and proposed control measures. That is, the model will calculate hourly ozone patterns likely to occur under the same meteorological conditions as the base case.

1.2   EMISSION INVENTORY REQUIREMENTS AND GENERAL PROCESSING METHODOLOGIES FOR PHOTOCHEMICAL MODELING

A photochemical model simulates the hour-by-hour photochemistry occurring for each grid cell in the modeling domain; consequently, the input emissions data must contain a comparable level of resolution. Total emissions (e.g., VOC, NO_x, $PM_{2.5}$) must be chemically allocated into the chemical classes employed by the model. Additionally, the emissions data must be spatially allocated by grid cell for each hour of the modeling episode. If photochemical modeling is being performed to evaluate potential control strategies, future-year inventories must be projected which incorporate anticipated changes in emissions levels. The following information was extracted from EPA's *Procedures for the Preparation of Emission Inventories for Carbon Monoxide and Precursors of Ozone, Volume II: Emission Inventory Requirements for Photochemical Air Quality Simulation Models* (EPA-450/4-91-014, May 1991). Refer to Table 2-2 of Section 2 for an internet link to emission guidance documents.

Spatial Resolution of Emissions

In order for a photochemical model to provide spatially resolved predictions of ozone and various other pollutants at the grid cell level, it must be supplied with emission data that have the same degree of spatial resolution (i.e., by grid cell). The amount of effort required to implement this resolution will vary depending on the type of source. Most existing data bases of point source emissions will contain location data for each source (typically reported to within a fraction of a kilometer), allowing direct assignment of emissions to the appropriate grid cells.

By contrast, spatial resolution of area source emissions requires substantially more effort. Two basic methods can be used to apportion area source emissions to grid cells. The most accurate (and resource-intensive) approach is to obtain area source activity levels for each grid cell. The alternative approach, more commonly employed, is to apportion the county-level emissions from the existing inventory to grid cells using some spatial surrogate indicator of emission levels or activity (e.g., population, census tract data, or type of land use). The major assumption underlying this method is that emissions from each area source behave spatially in the same manner as the surrogate indicator. In developing spatial apportioning factors, the emissions modeler should focus on determining accurate factors for the more significant sources. In most large urban areas local planning agencies can provide the emissions modeler with detailed land use, population, or in some cases, employment statistics at the subcounty level. The Census

Bureau also gathers and reports this type of data for the nation (generally at the subcounty level).

Because of the relative importance of highway motor vehicle emissions (which usually comprise a large fraction of total VOC and NO_x emissions for most urban areas), these sources should be considered separately from other area sources in the modeling inventory. Instead of using county vehicle miles traveled (VMT) or gasoline sales to estimate highway vehicle emissions (as annual and seasonal inventories sometimes do), urban transportation planning models should be employed to generate VMT on an individual link basis whenever possible. The emissions for each link could then be assigned to the appropriate grid cells based on link location coordinates.

Planning, land use, and transportation models are already in use in many urban areas, and can provide the emissions modeler with much of the data necessary to allocate area source emissions and develop emission estimates by link for highway motor vehicles. Such models may also be capable of forecasting emissions for use in the development of projected inventories. Local agencies (particularly metropolitan planning organizations, or MPOs) should always be contacted during the inventory planning process to determine what planning models are being used and how the data from these models can be used in developing an emission inventory. Independently developed information such as growth forecasts not only may be unnecessary but, when used in photochemical modeling, may be the basis for challenges to the modeling results because of alleged nonconformity with other projections available to the public.

Temporal Resolution of Emissions

In order to accurately predict hourly concentrations of ozone, a photochemical model requires hourly estimates of emissions for each grid cell in the modeling domain. The existing inventory from which the modeling inventory is developed will generally contain annual average or, for the peak ozone season, daily emission rates; the emissions modeler must adjust the emissions in the baseline inventory to reflect the conditions of the ozone episode being modeled, including seasonal adjustments for temperature or activity levels (if baseline emissions are reported as annual averages) as well as adjustments for the day of the week. In addition, they must be allocated to the hours of the modeling episode.

The most accurate approach for temporal distribution of emissions involves determining emission rates (or activity) for specific sources for each hour of a typical day in the time period being modeled. This approach is sometimes employed for point sources, but often proves impractical for all but the major sources in the region. More commonly, point source emissions are allocated by hour using the operating schedule information provided in the existing base-year inventory. Operating schedules for point sources are typically reported only in terms of hours per day, days per week, and weeks per year in operation, with seasonal variations reported in terms of percent of annual throughput. Consequently, the emissions modeler must determine the most representative allocation of emissions to the hours of the modeling episode. If possible, operational hours for major sources in the point source inventory should be obtained to supplement the operational information in the baseline inventory.

For area and mobile sources, the emissions modeler usually develops typical hourly patterns of activity levels for each source category. Typical temporal distribution profiles and adjustment factors for area and mobile source categories are available in the EPS3 distribution, however, these data may not be representative of a given region, which may differ significantly from national average profiles due to the effects of regional meteorological conditions or activity patterns.

Ideally, locale-specific temporal information should be collected for all sources that contribute significantly to the inventory. Regional weekday/weekend activity levels and diurnal variations by source category can be determined through special surveys or estimated using engineering judgment.

Chemical Resolution of Emissions

Since every reaction of all of the organic compounds found in an urban atmosphere cannot be considered, photochemical models generally group pollutants to limit the number of reactions and species to a reasonable level while permitting reasonable accuracy in predicting ozone formation. Photochemical models employ a chemical mechanism with a predefined set of air quality modeling compounds. Accordingly, VOC emissions must be disaggregated into chemical mechanism compounds prior to model application. These models require that NO_x emissions be disaggregated into NO and NO_2 and that $PM_{2.5}$ is disaggregated into the compounds that comprise particulate matter.

In the absence of more detailed information, VOC and particulate emissions can be speciated using the speciation profiles by source type contained in EPA's SPECIATE 4.0, Volatile Organic Compound (VOC)/Particulate Matter (PM) Speciation Data System (EPA/600/R-06/161, 2006). In some cases, however, source-specific speciation profiles or (less commonly) region-specific speciation profiles by source type may be available. If the latter are available, the factors associated with that source category can be modified to more accurately reflect the profiles of local sources. Issues the emissions modeler should consider when developing or modifying mechanism compound split factors include how hydrocarbon emissions are reported in the inventory (e.g., as VOCs, total hydrocarbons, reactive hydrocarbons, total non-methane hydrocarbons, etc.) and the compatibility of the speciation profile designations with the source classification scheme used in the inventory.

In some instances, data on VOC compounds for individual facilities may be available (perhaps through source tests or material composition considerations), and the emissions modeler may prefer to use these in the modeling inventory instead of an assumed VOC-compound distribution. Generally, however, most industries cannot provide reliable VOC or NO_x compound data or accurately apportion their emissions into appropriate chemical classes. Thus, typical VOC and NO_x distributions for various source categories are usually used. If speciation data are available for some facilities within the modeling domain, the emissions modeler must identify the correct chemical mechanism speciation of each individual hydrocarbon compound in the data. If splits for specific compounds in the speciated emissions data are unavailable, a photochemical modeling specialist familiar with both photochemistry and the chemical mechanism should be consulted to determine appropriate split factors for those compounds.

Development of Projected Inventories

There are basically two types of projections: baseline projections and control strategy projections. Baseline projections are estimates of future-year emissions that account for both expected growth in an area and air pollution control regulations that are in effect at the time the projections are made. If provisions in <u>existing</u> control regulations are to take effect at some future date, the baseline projections should include the effects of these expected changes. By contrast, control strategy projections also include the expected impact of <u>proposed</u> control regulations.

Two general methods can be employed for predicting future-year emissions levels: source-specific projections and aggregate projections. Information regarding projected increases in activity at existing facilities or proposed construction can be obtained directly from operators. Permit applications also provide a source of information about proposed expansions and new construction. Difficulties encountered in incorporating facility-specific projections into a modeling emissions inventory include differentiating between increased activity at existing facilities and increased activity due to new construction; for proposed facilities, the probable location, stack parameters, and operating schedules, as well as emissions, will need to be estimated for each point source within the facility.

Aggregate growth projections are more commonly employed in estimating future-year inventories. In some cases projection information may be available for types of point sources. Similarly, growth indicators may be employed to estimate future-year emissions for groups of sources. Local metropolitan planning offices regularly project demographic and economic parameters for planning purposes; such data can be used in place of or to supplement projections derived from national data.

Point source projections may be more difficult due to the problem of appropriately representing increased activity at each source. The emissions modeler has three basic options for allocating projected emissions changes for point sources:

1. Apply projected growth in each source category (e.g., electric utilities) equally across all existing plants in the county;
2. Apply projected growth in each source category across existing plants, weighing the growth more heavily in areas of the county targeted for greater industrial activity; or
3. Identify areas where new plant activities are scheduled to reflect growth due to the startup of new facilities as well as increased activity at existing facilities.

If the emissions modeler chooses to allocate projected emissions changes in industrially zoned land by grid cell rather than assuming that all increased activity will occur at existing facilities, hypothetical emission records for the proposed point sources must be developed. For area and mobile sources, the emissions modeler should review the surrogate indicators used to spatially allocate emissions in the base-year inventory and make any necessary modifications to account for anticipated changes in land use patterns or the existing transportation link network (e.g., proposed highway, railway, or airport construction). The user should refer to EPA's *Emission Inventory Improvement Program (EIIP) Document Series - Volume 10 Emissions Projections* (EPA, 1992) for additional guidance. Refer to Table 2-2 of Section 2 for an internet link to emission guidance documents.

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2. OVERVIEW OF THE EPS3 SYSTEM

EPS3 provides the user with expanded capabilities to support the CAAA requirements, conform to EPA emission inventory requirements, and provide a method for evaluating proposed control measures for meeting RFP regulations. Regulatory requirements call for hydrocarbon emissions to be reported as reactive volatile organic compounds and motor vehicle emissions to be adjusted hourly for temperature effects. EPS3 has features to process emission inventories that meet these requirements. Further capabilities include processing of a link-based emissions, point-specific speciation, and locale-specific temporal profiles.

The flexibility of EPS3 provides the user with many options for processing their emissions inventory. The design provides the users with (1) a "turn-the-crank" system for generating modeling inventories, and (2) a means for the discriminating user to implement detailed, locally available data such as source-specific speciation, temporal information, and episode specific emissions.

Typically, there are 4 tasks that must be performed on an emissions inventory to create emissions files for purposes of photochemical modeling:

1) convert reported criteria pollutants to model mechanism compounds (speciation)

2) project base year emissions to future years and/or apply controls to emissions to reflect current air quality legislation (growth and control)

3) convert annual (or period) emission rates to hourly emission estimates (temporal allocation)

4) allocate county level emissions to the modeling grid (gridding)

EPS3 consists of a series of FORTRAN modules that perform these intensive data manipulations, producing an emissions inventory for photochemical modeling. Each module is responsible for carrying out one of the necessary tasks.

2.1   CORE MODULES

The core EPS3 system (Figure 2-1) consists of the following modules, the primary functions of which are summarized.

PREPNT   Entry point for point sources; prepares the point source inventory for further processing, identifies which sources are to be treated as elevated by the photochemical model.

PREAM   Entry point for the area sources; prepares annual (or other period) county-level area and mobile source emissions for further processing.

LBASE   Entry point for the link-based motor vehicle sources; prepares link-based mobile source emissions estimates for further processing, allocates emissions to grid cells.

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2-1

PREFIR   Entry point for fire emissions reported as point sources; prepares the inventory for further processing, identifies the fire class of each source.

PRESHP   Entry point for shipping lane emissions; prepares the shipping emissions for further processing, allocates emissions to grid cells.

CNTLEM   Adjusts emissions levels to reflect the effects of anticipated growth or implementation of proposed controls.

CHMSPL   Assigns input hydrocarbon emissions to chemical compounds expected by the air quality model and disaggregates criteria pollutants into photochemical modeling compounds.

SPCEMS   Disaggregates criteria pollutants into photochemical modeling compounds based on speciation profiles of the air quality model chemical mechanism.

TMPRL   Temporally adjusts emissions from annual, seasonal, or typical season day to episodic levels; allocates emissions to the hours of the modeling episode.

PSTPNT   Screens the point source inventory and generates a stack list of elevated sources and emission inventory files to be processed by the PIGEMS module.

PSTFIR   Determines the fraction of fire emissions at the surface and determines the top and bottom of the plume for each source, generates a CAMx-ready surface emissions file and a stack list of elevated sources and emission inventory files to be processed by the PIGEMS module.

PSTSHP   Determines the distribution of shipping emissions to the vertical layers; generates a CAMx-ready surface emissions file and a stack list of elevated sources and emission inventory files to be processed by the PIGEMS module.

PIGEMS   Flags sources for Plume-in-Grid (PIG) treatment by the CAMx model, merges multiple elevated point source files, and generates a CAMx ready elevated emissions file.

GRDEM   Spatially allocates emissions based on source location, or gridded spatial surrogate indicators; generates a CAMx-ready surface emissions file.

MRGUAM   Merges multiple CAMx-ready surface emissions files into one file (e.g., merges anthropogenic and biogenic low-level emissions into the final CAMx-ready inventory of surface sources).
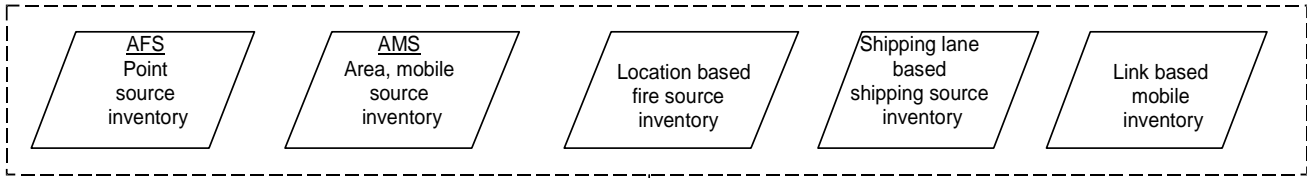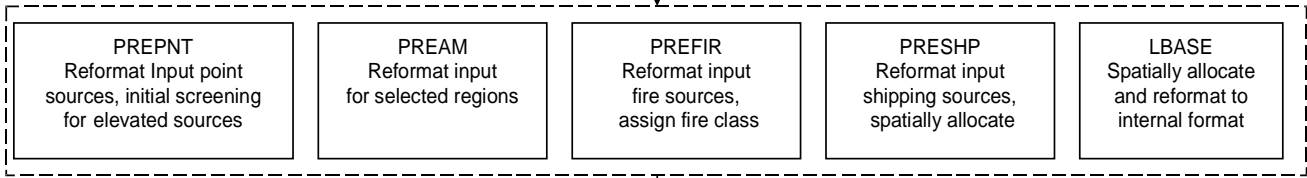
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Inventory Inputs
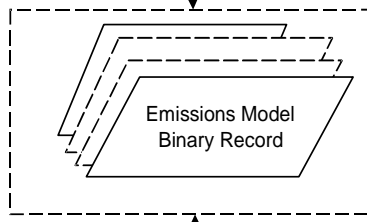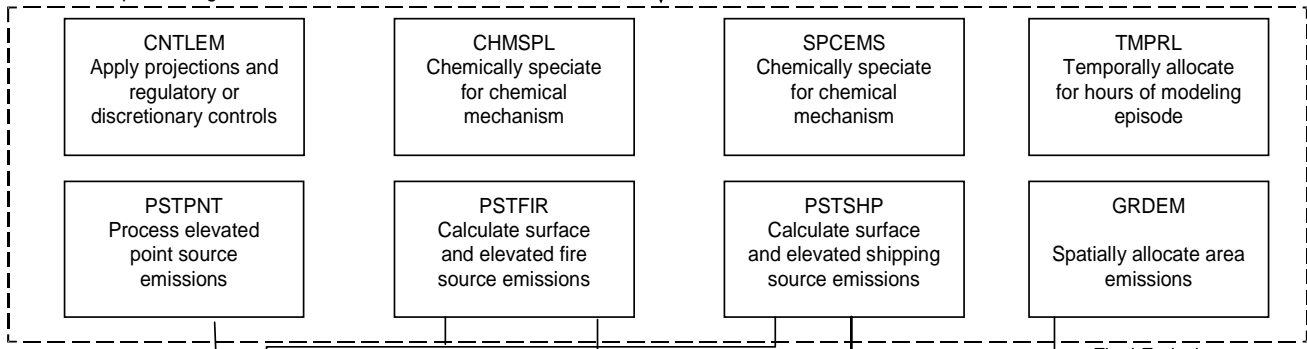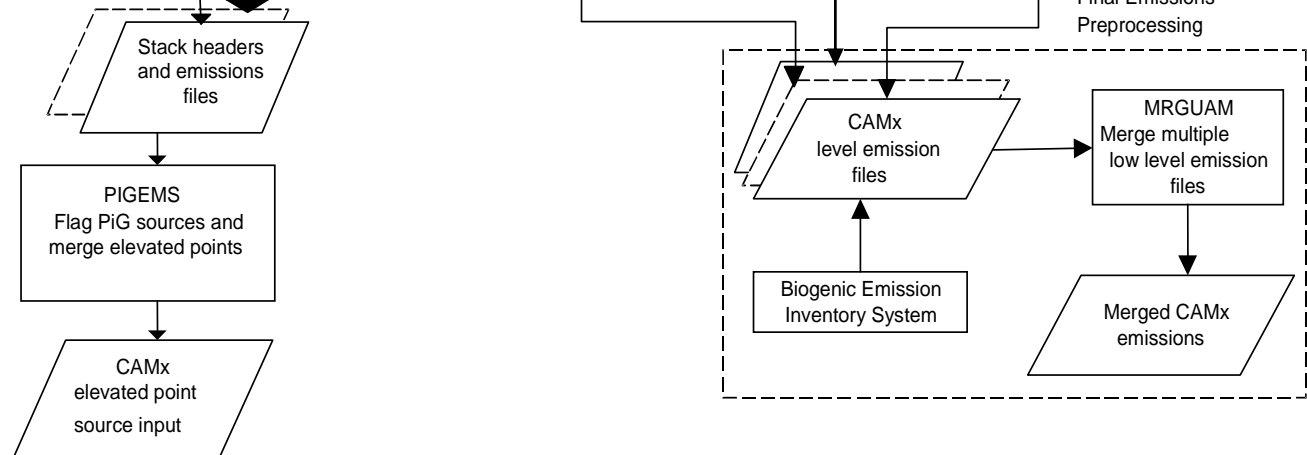
Figure 2-1. Overview of the emissions processing system (EPS3).

In general, point, area, and mobile source emission data should be processed separately in the EPS3 system to facilitate both data tracking for quality control and the use of the data in evaluating the effects of alternative proposed control strategies on predicted air pollutant concentrations.

The PREPNT, PREAM, PREFIR, PRESHP and LBASE modules serve as entry points to the EPS3 system for point source, area and mobile source, location specific fire source, shipping lane shipping sources, and link-based mobile source data, respectively; these programs must be executed to convert the input emissions data to the EPS3 internal Emissions Model Binary Record (EMBR) format, described in Section 2.7. Certain other modules may be executed in any order: CNTLEM (which simulates the effects of controls or growth), CHMSPL or SPCEMS (which speciates emissions into the chemical mechanism compounds required by the photochemical model), TMPRL (which temporally allocates emissions to the hours of the modeling episode), and GRDEM (which spatially allocates emissions to the grid cell of the modeling domain). If the GRDEM module is executed prior to execution of the other listed modules, the user must re-execute GRDEM in order to convert the gridded, speciated, hourly EMBR file to CAMx format.

> ➤ **Recommended Order of Execution for the EPS3 Modules to Minimize Computational and Data Storage Requirements.**
>
>   (1)   The entry modules (PREPNT, PREAM, PREFIR, PRESHP and LBASE);
>
>   (2)   CNTLEM, CHMSPL or SPCEMS, and TMPRL; because the TMPRL module produces hourly emissions estimates the output produced by TMPRL will typically be significantly larger than that of the other modules;
>
>   (3)   GRDEM;
>
>   (4)   PSTPNT for point source emissions (this module cannot be executed before TMPRL and CHMSPL);
>
>   (5)   PSTFIR for point specific fire source emissions, PSTSHP for shipping emissions;
>
>   (6)   MRGUAM, if multiple CAMx formatted files need to be merged for modeling; and
>
>   (7)   PIGEMS, if the PiG option is not utilized, this module merges multiple point source files and serves as a reformatter.
>
>   Spatial allocation of county-level emissions (performed by GRDEM) increases the size of the internal EMBR file by an order of magnitude. In some cases an input record containing the county-total emissions from a single source category can potentially be disaggregated into hundreds of gridded records. This is especially true when processing emissions for counties in the western United States, where counties may be quite large. Accordingly, it is recommended that spatial allocation be performed late in the EPS3 process to (1) reduce computing resource requirements, and (2) minimize the impact of any last-minute changes in the modeling region definition on inventory processing.

Point source data are initially processed by PREPNT, which performs an initial screening of the data to determine whether each source will be treated as low-level or elevated. PREPNT also converts the input data to the Emission Model Binary Record (EMBR) format (see Section 2.7). The point source inventory is then ready for temporal allocation and chemical speciation.

County-level area and mobile source emissions data enter the EPS3 system through the PREAM module. If data for calculating link-based mobile source emissions are available, the LBASE module serves as the entry point for these data. And similarly, if point-specific fire source emissions are available, the PREFIR module serves as the entry point for these data and for shipping lane emissions PRESHP is the entry module. The emissions files created by PREAM, and the other EPS3 entry modules, are in the EMBR format. Each EMBR file (area sources, onroad motor vehicle, nonroad motor vehicles, and point sources) is processed separately through the remaining modules of EPS3 to facilitate quality control tracking and control strategy analysis. Each file is chemically speciated by the CHMSPL or SPCEMS modules and temporally allocated by the TMPRL module. For area sources and motor vehicles, county-level emission totals by source category are spatially allocated to individual grid cells in the modeling domain by the GRDEM module; point source and point specific fire source emissions are allocated to grid cells based on source location. The GRDEM module has a user option for specifying the output emissions file format, either CAMx low-level emissions file format or gridded EMBR format. The final step in generating the model-ready input surface emissions file is the MRGUAM module which merges the multiple CAMx emissions files into a single model-ready file. The final merge should include biogenic emissions, which are discussed in Section 2.3. The final step in generating the model ready point source emissions is the PIGEMS module.

2.2   EPS3 UTILITIES

EPS3 includes support utilities that (1) generate some of the input files required by EPS3 core modules (2) allows review of the internal EMBR file data and (3) provides gridded chemical species for plotting. A list of the utilities and their purposes is provided in Table 2-1. A full discussion of each program is provided in Section 4. Utility Descriptions.

Table 2-1. EPS3 utility programs.

Utility	Input Files	Purpose
Input Preparation Support		
EMSCVT	Chemical mechanism compound database and profile definitions	Creates CHMSPL speciation profiles and optional source category cross-reference
TMPFAC	Point source emission inventory and optional SCC(ASC) temporal profiles cross-reference	Generates TMPRL module temporal profiles and updated profile cross-reference
EMBR Support		
EMBRET	EMBR - EPS3 internal binary file	Converts binary to ASCII for quality control and review
Output Support		
SPLTEM	Compressed EMBR and profile data	Generates gridded ASCII files

The EMSCVT and TMPFAC utilities generate the files expected by EPS3 CHMSPL and TMPRL modules. Default input data are often available from State and Federal agencies, though these data may need to be reformatted to EPS3 required formats. Links to these data and EPA emission inventory guidance documents are provided in Table 2-2.

The EMBRET utility operates on the EMBR file. It reads EMBR, written in machine-dependent binary format, and writes the data in ASCII format for user review. EMBRET will convert the

entire file or a subset of records based on user parameters. The EMBRET utility is useful for quality control purposes allowing a user to examine the individual data records.

The SPLTEM utility operates on a compressed EMBR file utilizing speciation profile data. It generates gridded emissions for chemical compounds (e.g. propylene) and criteria pollutants.

Table 2-2. Internet links to emission support documents and inputs as of August 2007.

EPA Emissions Guidance	
National Ambient Air Quality Standards for Ozone	http://www.epa.gov/groundlevelozone/fs20070620.html
State Implementation Plan (SIP) Attainment Demonstration Guidance	http://www.epa.gov/scram001/guidance_sip.htm#8ozone
Modeling Guidance and Support	http://www.epa.gov/scram001/guidanceindex.htm
Technical Support Documents, Reports and Journal Articles	http://www.epa.gov/scram001/reports/EPA-454-R-07-003.pdf
Technical Transfer Network	http://www.epa.gov/ttn/
EPA Emissions Modeling Clearinghouse	
Temporal Allocation	http://www.epa.gov/ttn/chief/emch/temporal/
Spatial Allocation	http://www.epa.gov/ttn/chief/emch/spatial/
Speciation	http://www.epa.gov/ttn/chief/emch/speciation/
Projection	http://www.epa.gov/ttn/chief/emch/projection/
Biogenic Emissions	http://www.epa.gov/ttn/chief/emch/biogenic/
Emission Inventory Related Codes	http://www.epa.gov/ttn/chief/codes/index.html#scc
EPA Emission inventories	
Clean Air Markets – Data and Maps	http://camddataandmaps.epa.gov/gdm/
National Emissions Inventories for the U.S.	http://www.epa.gov/ttn/chief/net/index.html
North American Emissions Inventories - Canada	http://www.epa.gov/ttn/chief/net/canada.html#data
North American Emissions Inventories - Mexico	http://www.epa.gov/ttn/chief/net/mexico.html
EPA Other	
Clearinghouse for Inventories & Emissions Factor	http://www.epa.gov/ttn/chief/ap42/index.html
Technology Transfer Network (TTN)	http://www.epa.gov/ttn/index.html
Selected AQS Code Description	http://www.epa.gov/ttn/airs/airsaqs/manuals/codedescs.htm
Other	
U.S. Census County Codes	http://www.census.gov/geo/www/fips/fips65/download.html

2.3   DATA REQUIREMENTS

The EPS3 system requires a variety of input data, which can be classified into five categories:

    Emissions data,
    System default parameters,
    Region-specific data,
    Episode-specific data, and
    Optional data.

Details regarding the content and format of the required input files for each EPS3 module and utility are addressed in Section 3 for core modules, and Section 4 for utilities; this section presents an overview of the general data requirements for EPS3.

Emissions Data

The user must supply the input emission inventory data that the EPS3 requires to process the modeling inventory. Before processing the emission data, the user should confirm that the inventory data is appropriate for the purposes of the modeling application. For example, an inventory used for model performance evaluation should reflect actual emission rates for the year of the modeling episode.

EPS3 supports emissions data in distinct file formats for: point sources, area sources, location specific fire sources, shipping lane shipping sources, and link sources. The point source data includes physical stack parameters, operating schedule, and emission values. The area source emissions file format is used for small stationary sources not included in the point source data, and both off-road and on-road motor vehicles. This format includes emission values by county and source category code. The location specific fire source data are daily emission estimates by location, similar to a point source. Instead of point stack parameters, the virtual acreage of the fire is specified. The shipping lane shipping sources specify emissions The link source data, typically for on-road transportation network data, includes link node coordinates, source category code (indicates fuel, vehicle class, facility class and mode), and emission values.

As stated above, the user must supply the emission inventory data for the EPS3 system. These data may either be retrieved from the National Emission Inventory (NEI) system or developed independently by the user; in either case the emissions data files must be formatted according to the required input format of each EPS3 module. For point source data the AIRS Facility Subsystem (AFS) work file format is required and for area and mobile source data the AIRS Area and Mobile Subsystem (AMS) work file format is required. The AFS and AMS work file formats are described in Tables 3-2 and 3-4, respectively, in Section 3: Core Modules.

The AFS work file contains the point source data required by the EPS3 to process this portion of the inventory. The information in the AFS work file can be divided into six types: inventory period, geographical, source identification, stack characterization, operating schedule information, and emission estimates. Table 2-3 lists the individual data items contained in the AFS work file for each of these six categories.

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Table 2-3. Types of data included on each record in the AFS work file.

Inventory Description Data	Stack Characterization Data

➢ Inventory period:
  Annual
  Typical peak ozone season weekday
  Typical peak CO season weekday
  Average day
  Other specified interval
➢ Period starting and ending dates and times
	Height (meters)
	 Diameter (meters)
	 Exit gas temperature (degrees Kelvin)
	 Exit gas velocity (meters per second)

Geographical Data ➢ FIPS state and county codes Subregion code (FIPS city code) (optional) ➢ Source location (geodesic, UTM or LCP) ➢ UTM zone (only required if source location is specified in UTM coordinates)	**Operating Schedule Information (optional)** Seasonal percentages of annual throughput Hours per day in operation Days per week in operation Hours/year in operation Start hour
Source Identification Data ➢ Plant identification code ➢ Stack identification code Point identification code Segment identification code ➢ Standard Industrial Classification Code (SIC) ➢ Source Classification Code (SCC)	**Emissions Data** ➢ Pollutant code ➢ Emissions for specified pollutant

Arrows (➢) indicate fields that must contain valid data for use in EPS3. Missing data in other fields will be replaced with default values or ignored.

> ➢ **Note**
> The user must know how pollutants are reported in the emissions data.
> In particular, whether hydrocarbons are reported as VOC or as TOG.
> Care must be taken to provide EPS3 with the inputs to correctly
> speciate the emissions into the proper chemical compounds.

Data fields (denoted in the table with an arrow, ➢) must contain valid data for use in EPS3. Although missing data in other fields will be replaced with default values, the resultant modeling emission inventory will be less accurately resolved which will, in turn, affect the quality of the CAM$_X$ modeling results.

> ➢ **Importance of Valid Data**
> The stack characterization data and operating schedule information
> should contain valid data for a majority of the records in the AFS file to
> ensure that (1) elevated sources will be correctly identified and modeled,
> and (2) emissions will be accurately allocated to the hours of the
> modeling episode. Although the EPS3 system can, in some cases,
> replace missing or invalid data with defaults, it is recommended that the
> user provide valid data for all fields. Of particular concern is the operating
> schedule information. If provided, the TMPFAC utility can be run to
> update the default temporal allocation files to include the source specific
> information. If this data is not available, the TMPRL module will use the
> system defaults, which may not be appropriate for the specific
> application.

Table 2-4 lists the data items contained in the AMS work file for area and mobile sources. The data in this file can be divided into four categories: inventory description, geographical, source identification, and emissions. Data fields that must contain valid data for use in EPS3 are denoted with an arrow (➢).

Table 2-4. Types of data included on each record in the AMS work file.

Inventory Description Data	Geographical Data
➢ Inventory period: Annual Typical peak ozone season weekday Typical peak CO season weekday Average day Other specified interval ➢ Period starting and ending dates and times	➢ FIPS state and county codes Subregion code (FIPS city code) (optional) **Source Identification Data** ➢ Area Source Category code **Emissions Data** ➢ Pollutant code ➢ Emissions for specified pollutant

Arrows (➢) indicate fields that must contain valid data for use in EPS3. Missing data in other fields will be replaced with default values or ignored.

Biogenic Emissions

Biogenic emissions have proven to be an important component of the emissions data needed to predict ozone using a photochemical model. Biogenic emissions are estimated using a stand-alone model. The resulting emissions inventory is then formatted for input to CAMx then incorporated into the inventory using the EPS3 module, MRGUAM. Several biogenic emission models are available. Table 2-5 lists the aspects of each model and provides an internet address if available.

Table 2-5: Biogenic Emissions Models.

Model	Emission Factor Algorithm	Landcover Data	Chemical Mechanisms Supported	Programming Language/Operating System
CONCEPT[a]	BEIS3, MEGAN	BELD 3.1[e], MEGAN	CB-IV, CB05, SAPRC99	SQL/Windows, Linux
GloBEIS[b]	BEIS3	BELD 3.1 or other	CB-IV, CB05, SAPRC99	MS Access/Windows
SMOKE[c]	BEIS3	BELD 3.1	CB-IV, SAPRC99	FORTRAN/Linux
MEGAN[d]	MEGAN	MEGAN	CB-IV, CB05, SAPRC99	FORTRAN/Linux

a) http://www.conceptmodel.org
b) http://www.globeis.com
c) http://www.smoke-model.org
d) http://bai.acd.ucar.edu/Megan
e) The BELD version 3.1 database provides landcover data for North America with 1 km spatial resolution. Processing is required (e.g., using a GIS) to format the data for use with biogenic emission models.
f) MEGAN has global landcover data with 1 km spatial resolution. Processing is required (e.g., using a GIS) to format the data for use with the MEGAN or CONCEPT emission models.

System Default Parameters

EPS3 comes with a set of files containing default inputs for certain data, which are intended to provide the user with an initial EPS setup. These files include:

Speciation profiles for chemically allocating the emissions to the chemical mechanism compounds used by the CAMx model (derived from data in EPA's *SPECIATE 4.1*),

Speciation profile code assignments by Source Classification Code (SCC) and Area Source Category (ASC) code,

National average temporal allocation profiles, and

Temporal profile code assignments by SCC (ASC).

In the absence of source- or region-specific data the default speciation profiles, speciation profile assignments and temporal allocation data represent EPA-preferred data sources for speciation and operating schedule data, respectively. The user should review all default inputs for appropriateness for each application. Internet links to EPA web sites which provide access to the default data are listed in Table 2-2.

> ➢**Use of Default Files**
> Of the default files, the two temporal allocation files have perhaps the least adequate information for any given EPS3 application, particularly for point sources. Specific operating schedule information from the AFS file should be incorporated in the temporal allocation profiles and source/temporal profile code assignments. This can be achieved with the TMPFAC utility.

Region-Specific Data

The user must specify the region to be modeled in the /REGION/ packet of the global USERIN user-input file, described in Section 2.4. Items the user must supply include;

Domain reference origin coordinates,

UTM zone (valid when origin coordinates are UTM),

Grid origin (in kilometers from the reference origin), and

Grid cell size and number of grid cells in the X and Y directions.

EPS3 requires this information to identify which input emissions data records are in the modeling domain and to spatially allocate emissions over the modeling grid.

To spatially allocate area and mobile emissions to the grid cells of the modeling domain, the user must also supply a file containing gridded surrogate data. The gridded surrogates determine how a county-level emissions source is to be allocated to the modeling grid. Known measurable quantities, such as population or urban land use, are used as surrogates for the activity producing the emissions for a given source category. This measurable quantity is allocated to the grid cells in a given county (gridded) and is used to represent the spatial distribution of the emissions source. The GRDEM module, described in detail in Section 3, provides the details for the gridded surrogates file. EPA has access to a national land use data base and can provide gridded spatial allocation surrogate data for specific areas or modeling domains upon request.

Any region-specific inputs that the user considers more appropriate than the default inputs provided with the EPS3 distribution should be used (e.g., locally developed demographic or region-specific speciation or temporal profiles that account for differing operating practices in various areas).

Episode-Specific Data

The episode to be modeled and the number and names of the chemical mechanism compounds are defined in the USERIN packets /DATE/ and /SPECIES LIST/, respectively. This information may be obtained from the CAMx modeler. The episode begins at the first hour and continues to the end of the last hour. To process an entire day the beginning hour is specified as "00" and the ending hour as "24." Since EPS3 processing is limited to a time span of 24 hours, only one date in calendar format is entered. The format of the date, which should represent the calendar date, is "YYMMDD", where "YY" is the year, "MM" is the month and "DD" is the day. For example an inventory for August 13, 1999 would be entered "990813." EPS3 will convert the calendar date to the Julian format required in the model-ready input files.

> ➤ **Daily Emissions Inventory Files**
> Although EPS3 is designed to generate a file for each of the days in the modeling episode, it is standard practice to produce a set of "representative" days for the modeling episode. Typically the representative days include a weekday, a Saturday and a Sunday for each of the four seasons: Winter, Spring, Summer and Fall. Representative days can be used in this way because the temporal allocation of sources is typically constant during a seasonal period and only has weekly variation for the weekend days. Using representative days can greatly reduce the amount of processing time and disk space needed for a modeling application. However, introducing any daily specific parameters into the inventory processing, such as temperature adjustments to motor vehicle sources, will necessitate an individual processing stream for each day of the modeling episode.

Optional Data

Optional inputs to the EPS systems include link-based motor vehicle emissions data, fire emission estimates, shipping lane emissions, source-specific temporal data, source-specific chemical composition data, and special inventories.

2.4 USERIN, THE EPS3 USER INPUT FILE

Each of the core EPS3 modules accesses the user input file, referred to as the USERIN file. The USERIN file consists of a number of sections, referred to as *packets*. Each packet begins with an identifier keyword(s) enclosed in forward slashes "/*packet name*/" and terminates with the keyword "/END/." These packets contain the input parameters that are application specific, such as: output message file options, default parameters, region description, modeling episode description, and others. Together, these parameters tell the EPS3 system how to handle the input data and what type of inventory to produce. Most of the core modules in the EPS3 system require a module-specific packet in the USERIN file, defining the input parameters for that module. The module-specific USERIN packets are described in detail in Section 3. Each module reads only those packets that contain information needed for that module. The USERIN file is an EPS3 system-wide file. One USERIN file may be set up for an entire EPS3 application, to be used with all modules. A module will search the entire USERIN file for the necessary packets, which can occur in any order. In most cases, the first 20 characters of any line in a USERIN packet are ignored. This space is typically used to provide a brief description as to what data value is expected on that particular line. The descriptions are for reference purposes

only; they are ignored by the EPS3 modules. In addition, the USERIN file can be annotated by adding notes outside packets. All records outside of a packet are ignored by the EPS3 modules.

In addition to the module-specific packets, the USERIN file contains packets that describe the modeling setup, emissions characteristics, and output table options. Modeling setup packets provide the mechanism for the user to define the time period of the episode, the modeling domain and geographical area coverage.

The following packet keywords define a model run and are read by multiple EPS3 modules:

/DATE/	episode definition
/REGION/	modeling region definition
/COUNTY/	county list
/CRITERIA POLLUTANT/	input pollutants to be modeled
/SPECIES LIST/	modeling compounds
/CRITERIA TABLES/	output report tables
/SPECIES TABLES/	output report tables

A detailed description and field formats are provided below for each of these general USERIN packets.

/DATE/　　　　This packet defines the time period of the episode (Table 2-6); Exhibit 2-1 shows a sample /DATE/ packet for a CAM_X application. EPS3 expects the date in calendar format ("YYMMDD").

Table 2-6. /DATE/ packet fields of USERIN.

Line	Columns	Type	Description
1	1-20	C	Packet identifier - /DATE/
2	1-20	C	Label (ignored)
	21-80	C	Inventory Identification Note (arbitrary string)
3	1-20	C	Label (ignored)
	21-30	I	Inventory date (yymmdd)
4	1-20	C	Label (ignored)
	21-30	I	Beginning time (00 – first hour of the day)
5	1-20	C	Label (ignored)
	21-30	I	Ending time (24 – last hour of the day)
6	1-20	C	Packet terminator - /END/

```
/DATE/
Inventory Note      :CAMx Modeling extended regional, 8/13/99
Inventory Date      :990813
Beginning Time      : 0
Ending Time         : 24
/END/
```

Exhibit 2-1. DATE packet of USERIN.

/\REGION/   This packet defines the modeling region and grid resolution (Table 2-7). Exhibit 2-2 shows an example /REGION/ packet. The packet includes the number of cells in the modeling grid, cell size, and modeling domain origin. The units are kilometers for UTM or LCP, and decimal degrees for Geodesic coordinates.

Table 2-7. /REGION/ packet fields of USERIN.

Line	Columns	Type	Description
1	1-20	C	Packet identifier - /REGION/
2	1-20	C	Label (ignored)
	21-30	R	Origin coordinate in X direction
	31-40	R	Origin coordinate in Y direction
3	1-20	C	Label (ignored)
	21-30	I	UTM zone (0 for non-UTM coordinates)
4	1-20	C	Label (ignored)
	21-30	R	Cell width in X direction
	31-40	R	Cell width in Y direction
5	1-20	C	Label (ignored)
	21-30	I	Number of cells in X direction
	31-40	I	Number of cells in Y direction
6	1-20	C	Packet terminator - /END/

```
/REGION/
Domain Origin      :-108.0     -1584.0
UTM Zone           :0
Cell Width         :36.0        36.0
Number of Cells    :69          67
/END/
```
Exhibit 2-2. REGION packet of USERIN.

/COUNTY/   This packet contains a list of the counties in the modeling region (Table 2-8). Exhibit 2-3 shows an example /COUNTY/ packet. Data from any county other than those in the county list will not be processed. Each county is identified by a *Federal Information Processing Standards* (FIPS) state/county code. The first 20 columns of each county line are optional identifiers and can be used to specify the name of each county (EPS3 does not read this information). Each county line also contains a field for identifying the time zone of the county. The time zone flag is used to shift the emissions activity from the time zone of the county to the time zone of the modeling application. Because the CAMx model must be run using a fixed time zone, it is necessary to adjust the temporal distribution of emissions in any county where the time zone does not match the time zone used in the modeling application. The EPS3 distribution includes a file containing an entry for each county (or parish) in the United States.

Table 2-8. /COUNTY/ packet of USERIN file.

Line	Columns	Type	Description
1	1-20	C	Packet identifier - /COUNTY/
2+	1-20	C	Name of county (optional)
	21-25	C	FIPS code of state/county
	27-36	C	Time zone
3	1-20	C	Packet terminator - /END/

```
/COUNTY/
Anderson, TX        :48001  CST
Angelina, TX        :48005  CST
Aransas, TX         :48007  CST
.
.
.
Young, TX           :48503  CST
Zapata, TX          :48505  CST
Zavala, TX          :48507  CST
/END/
```
Exhibit 2-3. COUNTY packet of the USERIN file.

The characteristics and chemical composition of the input emission data is provided by the user. EPS3 does not assume default information with regard names, codes, or chemical speciation split factors. The user has the responsibility of providing this information.

/CRITERIA POLLUTANT/ This packet identifies the criteria pollutants included in the input emission inventories (read by PREAM, PREPNT, and PREFIR) that are to be included in the EPS3 modeling (see Table 2-9). Exhibit 2-4 provides an example of this packet. The pollutant name is used for reporting purposes and in some of the look up tables. The corresponding pollutant code is the input emission inventory code, historically represented by the SAROAD code. If a pollutant code in the input emissions file is not found in this packet, the record is skipped and the data is excluded from the modeling.

The order of the criteria pollutants in the packet is the order in which they are written to the message files. This packet information is carried in the header section of the EMBR file, and represents the order of emissions carried on the EMBR data records. Nothing internal to EPS3 modules requires a particular name or code, as such; the names and codes in this packet are somewhat arbitrary. It is recommended that the names and codes established by the EPA be used to identify the pollutants in the input inventory files.

Table 2-9 /CRITERIA POLLUTANT/ packet of USERIN file.

Line	Columns	Type	Description
1	1-20	C	Packet identifier - /CRITERIA POLLUTANT/
2+	1-20	C	Label (ignored)
	21-30	C	Name of criteria pollutant
	31-40	I	Pollutant code
3	1-20	C	Packet terminator - /END/

```
/CRITERIA POLLUTANT/
Nitrous Oxides    : NOx      42603
HydroCarbon       : VOC      43104
Carbon Dioxide    : CO       42101
Sulfur            : SOX      42401
Particulates < 10 : PM10     11101
Particulates < 2.5: PM25     81102
/END/
```

Exhibit 2-4. CRITERIA POLLUTANT packet of the USERIN file.

/SPECIES LIST/ This packet specifies the list of chemical mechanism compounds that are generated in the modeling inventory. These are the final output species/compounds. Compounds listed here are derived from the associated input inventory criteria pollutant and written to the model-ready emissions files. The compound (or species) name, associated criteria pollutant, and molecular weight are designated by the user (see Table 2-10). Exhibit 2-5 shows an example of this packet. The molecular weight is used to convert emissions estimates from moles to grams for purposes of reporting.

Table 2-10. /SPECIES LIST/ packet of USERIN file.

Line	Columns	Type	Description
1	1-20	C	Packet identifier - /SPECIES LIST/
2+	1-20	C	Label (ignored)
	21-30	C	Chemical mechanism compound name
	31-40	C	Parent criteria pollutant name
	41-50	R	Species molecular weight
3	1-20	C	Packet terminator - /END/

```
/SPECIES LIST/
              :NO        NOX        46.0
              :NO2       NOX        46.0
              :OLE       VOC        32.0
              :PAR       VOC        16.0
              :TOL       VOC       112.0
              :XYL       VOC       128.0
              :FORM      VOC        16.0
              :ALD2      VOC        32.0
              :ETH       VOC        32.0
              :MEOH      VOC        16.0
              :ETOH      VOC        32.0
              :ISOP      VOC        80.0
              :CO        CO         28.0
              :SO2       SO2        64.0
/END/
```

Exhibit 2-5. SPECIES LIST packet of the USERIN file.

All of the EPS3 modules produce output tables in a consistent format. In addition to a summary table of processed emissions, each module can produce a number of detailed output tables. The output tables to be generated by a module are specified in two packets:

/CRITERIA TABLES/ This packet designates which output tables to produce for the criteria pollutants (Table 2-11.) For an example see Exhibit 2-6.

/SPECIES TABLES/ This packet specifies which output tables to produce for the chemical mechanism compound species. This packet structure is identical to that of /CRITERIA TABLES/ in Exhibit 2-6 with the exception that /SPECIES TABLES/ replaces the keyword.

Table 2-11. /CRITERIA TABLES/ and /SPECIES TABLES/ packet of USERIN file.

Line	Columns	Type	Description
1	1-20	C	Packet identifier - /CRITERIA TABLES/ or /SPECIES TABLES/
2	1-20	C	County table label (ignored)
	21-30	C	EPS module names, separated by space or a comma
3	1-20	C	Source category table label (ignored)
	21-30	C	EPS module names, separated by space or a comma
4	1-20	C	County and source category table label (ignored)
	21-30	C	EPS module names, separated by space or a comma
5	1-20	C	Hour table label (ignored)
	21-30	C	EPS module names, separated by space or a comma
6	1-20	C	Source category and hour table label (ignored)
	21-30	C	EPS module names, separated by space or a comma
7	1-20	C	County and facility table label (ignored)
	21-30	C	EPS module names, separated by space or a comma
8	1-20	C	County, facility and stack table label (ignored)
	21-30	C	EPS module names, separated by space or a comma
9	1-20	C	County, facility, stack and point table label (ignored)
	21-30	C	EPS module names, separated by space or a comma
3	1-20	C	Packet terminator - /END/

```
/CRITERIA TABLES/
County              :
Source Category     : PREAM Tmprl
County and Src Cat :
Hour                : TMPRL,
Src Cat and Hour    :
County and Facility:
Cty, Fac and Stk    :
Cty, Fac, Stk, Pnt :
/END/
```
Exhibit 2-6. CRITERIA TABLES packet of the USERIN file.

The possible output tables and the order in which they are specified are provided below:

County
Source category
County and source category
Hour
Source category by hour
County and facility
County, facility and stack
County, facility, stack and point

To generate a table for a given module, the module name is added to the report-option line defining that type of table. The module names expected are PREAM, PREPNT, LBASE, PREFIR, CHMSPL, SPCEMS, TMPRL, GRDEM, PSTFIR, and PSTPNT. Any number of the module names can be included and in any order, using any combination of upper and lower case letters. Misspelled names will be ignored. Using the example shown in Exhibit 2-6, the PREAM module will generate a table of emissions by source category code and the TMPRL module will produce two tables, one by source category code and another by hour of the day. The tables will be written to the message file created by the module.

The /CRITERIA TABLES/ and /SPECIES TABLES/ packets can also be used to generate a comma-delimited (CSV) file containing the same data that is written to the message file. This allows the user to easily import the table into a spreadsheet program or database application. Following the module name by a comma (",") as shown on the Hour line in Exhibit 2-6, will cause a comma delimited (CSV) file to be generated for that module and that type of table. The filenames for the CSV files are created by appending an extension to the name of the message file for that run. The extensions are listed in Table 2-12.

Table 2-12. Comma delimited file name extensions.

Output Table	Extension
County (criteria)	.cnty.crt.csv
County (speciated)	.cnty.spc.csv
Source Category (criteria)	.asc.crt.csv
Source Category (speciated)	.asc.spc.csv
County and Source Category (criteria)	.cnty.asc.crt.csv
County and Source Category (speciated)	.cnty.asc.spc.csv
Hour (criteria)	.hrs.crt.csv
Hour (speciated)	.hrs.spc.csv
Source Category and Hour (criteria)	.asc.hrs.crt.csv
Source Category and Hour (speciated)	.asc.hrs.spc.csv
County/Facility (criteria)	.facility.crt.csv
County/Facility (speciated)	.facility.spc.csv
County/Facility/Stack/Point (criteria)	.point.crt.csv
County/Facility/Stack/Point (speciated)	.point.spc.csv
County/Facility/Stack (criteria)	.stack.crt.csv
County/Facility/Stack (speciated)	.stack.spc.cs

Be aware that although any table can be specified for any module, requesting a level of detail not yet available in the processing stream will not produce a meaningful table. For example, requesting an hourly output table prior to running TMPRL will produce a table in which the hourly distribution is a flat profile. That is, output details available are dependent on the processing steps already performed on the current EMBR file.

2.5   BEST MATCH CRITERIA

EPS3 allows the user to input both source-specific inputs and default inputs without the need for intensive data manipulation and processing. For example, if detailed speciation data are available for only a single source in the modeling domain, EPS3 allows the data to be used without requiring that all sources have data at the same level of detail.

In general, one or more of the following fields is used to identify an emissions source: FIPS state/county code, subregion code, SCC(ASC), and plant and stack identification codes. If the input data are to be applied to a specific source, then all fields that are applicable are specified. However, for an overall application of the input, the specific fields are either left blank or filled with zeros. The EPS3 system will use best match criteria to identify which data is to be applied to any given source. Specifically, the state/county FIPS code is of the form ssccc (ss-state, ccc-county), so a FIPS state/county code of 00000 can be used to indicate data for the entire modeling region. To identify all of the sources in a single state, use the global FIPS state code ss000, where ss is the two-digit code for the specified state. The ASC code has a similar hierarchical structure. Table 2-13 shows the best match criteria coding scheme used in EPS3.

Table 2-13. Description of best match criteria.

FIPS State/County Code	Matching Criteria	Example
00000	all counties	00000 = all counties
ss000	all counties in state ss	06000 = all of California
ssccc	exact match for county ssccc	06067 = Sonoma County, CA
ASC code	**Matching Criteria**	**Example**
0000000000	all source categories	0000000000 = all sources
nn00000000	all sources beginning with the first 2 characters nn	2200000000 = all motor vehicle sources
nnnn000000	all sources beginning with the first 4 characters nnnn	2260000000 = all 2-stroke gasoline off-road motor vehicles
nnnnnnn000	all sources beginning with the first 7 characters nnnnnnn	2260004000 = all 2-stroke gasoline lawn and garden equipment
nnnnnnnnnn	exact match	2260004010 = 2-stroke gasoline residential lawn mowers

Although the point source identification information does not have a hierarchical structure, the EPS3 system does incorporate best match criteria for the point source identification codes. For each of the point source identification codes (plant ID, stack ID, point ID and segment ID) a global code consisting of all blanks is used to match all sources. For example, to have a control factor apply to all stacks in a given facility, you specify the FIPS state/county code and plant ID for the facility, leaving all other identification codes blank.

2.6 ERROR HANDLING PROCEDURES

The core EPS3 modules identify three classes of errors, each resulting in a different type of error handling action by the module. In order of increasing severity, these actions are

    (1)   Skip the record that caused the error and continue processing at the next record;

    (2)   Write the record containing erroneous data to a separate output file and continue processing at the next record; and

    (3)   Abort execution.

Some reasons that cause emission data to be skipped include total input emissions below a minimum specified level or source location outside of the defined modeling region. Records

written to error output files fail to meet a more stringent set of conditions (e.g., failure to match required input cross-references, or omitted required input parameters). The PREPNT, PREAM, PREFIR, PRESHP. and LBASE modules create error data files output in the same format as the input record for each module; all other EPS3 modules produce error files in the Emissions Model ASCII Record (EMAR) format, described in Section 2.8.

Each module echoes the filename as it is read from the job script. The messages help the user to trouble shoot the runs. This feature is useful when setting up new job scripts. At the completion of a program, the number of non-fatal warning messages is written to the standard output file. The message at the end of the run looks like this:

```
Successful completion of EPS3 GRDEM module v. 3.02 Aug 2008
There were 3 warning messages written.
```

In the case of an abort, the message will look like this:

```
An error occurred while running EPS3 GRDEM module v. 3.02 Aug 2008
If no explanation is given above, check the message file for details.
```

The user should review any warnings written to the message file to determine the nature of the warnings and decide if they are significant enough to require user-intervention. In some cases, when the final emissions inventory is not significantly affected, the warning message can be ignored. It is easy to identify the warning messages within the message output file. Each warning will be surrounded by a line of slashes. An example of a warning message is shown below. Regardless of how many times a processing step triggers the warning; only one instance of a warning message is written to the message file.

```
/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\

WARNING: Header read from input file is not consistent with /EPISODE/ packet.
File: ../emiss/emiss.ar.all_reg.99powkd
Input EMISSIONS header:
        File note                     :CAMx Modeling ODEQ regional, 8/16/99
        Beginning date                :99225
        Beginning time                :   0.00
        Ending date                   :99225
        Ending time                   :  24.00


/EPISODE/ header:
        Beginning date                :99228
        Beginning time                :   0.00
        Ending date                   :99228
        Ending time                   :  24.00


/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\
```

The most serious error condition, termination of the program, usually occurs when the specified inputs will not allow proper processing of data. The following list gives examples of conditions resulting in each of the three actions.

Skip record
> Total emissions for all criteria pollutants below limit
> Input county not included in /COUNTY/ packet of USERIN file
> Point source located outside of defined modeling domain

Write erroneous data record
> Missing stack parameters and user has selected not to assign defaults
> No match of input field in cross reference
> Missing or unexpected pollutant code (PREPNT, PREAM, PREFIR, LBASE)

Abort execution
> Inconsistent species list
> I/O error on read, write, open
> Missing required packet
> No match on requested species
> Required input file empty
> Input data parameters exceed module array bounds
> Invalid user option
> Required processing step skipped (GRDEM, PSTPNT, PSTFIR)
> Modeling region definition mismatch (MRGUAM)

2.7 THE EMISSIONS MODEL BINARY RECORD (EMBR) FORMAT

The Emissions Model Binary Record format, or EMBR, is an internal file format common to all of the EPS3 modules. The EMBR file is a binary file containing three types of records: (1) header records, (2) data records and (3) a trailer section. Each of these is discussed in detail below. The variables for the EMBR format are described in Table 2-14.

Each data field in an EMBR file may contain either a valid value or a flag indicating a missing value. The "missing value" flag is a blank for a character field, a "-9" for an integer field, and a "-9.0" for a real field. The same field may have valid data in one file and a missing value flag in another, depending on both the stage of processing (i.e., the modules that have been executed) and the type of data contained in the EMBR file (point, area, mobile, or combined). For example, the fields for stack information will have missing value flags in a motor vehicle data record.

Header Records

The first section of an EMBR file consists of a series of header records, which indicate the type of data in the file, the modeling region definition, the chemical mechanism compounds being employed, and a processing history.

The first record specifies the file type, which describes the type of data contained in the file. The file type for a particular EMBR file is assigned by the system entry modules. PREPNT assigns "POINTS", PREAM assigns "AREA", LBASE assigns "MOBILE", PREFIR assigns "FIREPTS", and PRESHP assigns "SHIPS".

The header record specifying modeling region definition may or may not contain information, depending on whether the file has been gridded. The region definition header includes the origin

coordinates, UTM zone (when needed), number of grid cells in the north-south and east-west directions, and grid cell size.

Because EPS3 supports a variable pollutant list, a header record is used to identity which pollutants are included in the inventory and in which order they appear in the file. This information is taken from the /CRITERIA POLLUTANT/ packet of the USERIN file and written to the EMBR file by the entry modules.

The header records which list the chemical mechanism compounds and molecular weights are written to the EMBR file after the data have been chemically speciated by the CHMSPL or SPCEMS modules. This section of the EMBR file also indicates the criteria pollutants from which these species were derived (VOC, NO_x, etc.). The last set of header records for each EMBR file provides a history of the EPS3 processing up to that point. Each EPS3 module previously run on that file is listed with the date and time of execution.

Table 2-14. Emissions Model Binary Record (EMBR) file contents.

Record	Variable	Type/Size	Description
Header Records			
1	FILTYP	C30	File Type: POINTS AREA MOBILE FIREPTS SHIPS
2	STRING	C	Input string internally formatted:
	RGUTME	F10.4	Region origin "X" coordinate (km or decimal degree).
	RGUTMN	F10.4	Region origin "Y" coordinate (km or decimal degree)
	IRGZN	I10	Region UTM zone (optional if geodesic)
	NXRGN	I10	Number of grid cells in east-west direction
	NYRGN	I10	Number of grid cells in north-south direction
	DXRGN	F10.4	Grid cell size (km)
	DYRGN	F10.4	Grid cell size (km)
3	NCRTHD	I10	Number of criteria pollutants
	NSPCHD	I10	Number of chemical species
4	CRTNAM(1)	C10	Criteria pollutant name
	ISAROD(1)	I10	Input inventory pollutant code
	. . .	. . .	. . .
	CRTNAM(NCRTHD)	C10	Criteria pollutant name
	ISAROD(NCRTHD)	I10	Input inventory pollutant code
5	SPCLST(1)	C10	Species name
	MOLWT(1)	R	Molecular weight of species
	SPCRIT(1)	C10	Criteria pollutant name generating the species
	. . .	. . .	. . .
	SPCLST(NSPCHD)	C10	Species name
	MOLWT(NSPCHD)	R	Molecular weight of species
	SPCRIT(NSPCHD)	C10	Criteria pollutant name generating the species
6+	PRGNM	C40	Program name and version number
	EXDAT	C	Date program executed
	EXTIM	C	Time program executed

Table 2-14. Emissions Model Binary Record (EMBR) file contents (concluded).

Record	Variable	Type/Size	Description
Data Records			
9	KEYWRD	C10	Keyword indicator - [DATA]
10+	FIP	C5	FIPS state/county code
	SBRGN	C5	Subregion code
	SICCD	C4	Standard Industrial Classification Code
	SCCCD	C10	Source Category Code (ASC)
	RECTYP	C1	Record type: 'E' = elevated point 'L' = low level point 'M' = mobile source 'F' = fire source 'S' = shipping source ' ' = stationary area source
	PERIOD	C2	Input inventory period type, e.g., PO
	INVBEG	I	Beginning Julian date/time (YYDDDHH)
	INVEND	I	End Julian date/time (YYDDDHH)
	IJCELL	I	Cell location of gridded inventory
	PLANT	C10	NEDS Plant Identification code
	ISTACK	C10	Stack Number
	POINT	C10	Point identification
	ISEGNO	C3	Segment Number
	UTME	R	UTM Easting Coordinate (km) to define location of plant
	UTMN	R	UTM Northing Coordinate (km) to define location of plant
	IUTMZN	I	UTM zone
	STKGEV	R	Stack Exit Gas Velocity (m/s)
	STKDIA	R	Stack Diameter (m)
	STKTMP	R	Stack Exit Gas Temperature (K)
	STKHGT	R	Stack Height (m)
	EMIN(1) … EMIN(NCRTHD)	R R	 Emissions (tons) for criteria pollutants
	SPCPOL(1) ... SPCPOL(NSPCHD)	R R	 Emissions (moles) for speciated pollutants
11	KEYWRD	C10	Keyword indicator - [TRAILER]
12	INRECS	I	Number of DATA records in this EMBR file
			Repeated for each process performed on file:
13+	PNAME	C30	Program name
	NFIN	I	Number of input files for program PNAME
	NFOUT	I	Number of output files for program PNAME
14+	FILIN	C80	Input file names
15+	FILOUT	C80	Output file names
16	TOTIN	R	Input totals to PNAME for criteria pollutants
17	TOTOUT	R	Output totals from PNAME for criteria pollutants

Data Records

Following the header section of the EMBR file are the emissions data and other source information necessary for processing; the beginning of this section has the identifying keyword "/DATA/." Each data record contains the following types of information.

Record type: "E" for elevated point source, "L" for low-level point source, "M" for mobile source, "F" for fire source, "S" for shipping source, or blank for area source.

Geographical information: FIPS state and county codes, subregion code (optional), facility location (for point sources and location specific fire sources), and grid cell coordinates if the file has been gridded.

Episode specification: beginning and ending dates and times for which the data is valid.

Source identification: plant identification code, point identification code, stack, and segment number (for point sources only); Standard Industrial Classification (SIC) code; Source Classification Code (for point sources) or Area Source Category code (for area and mobile sources).

Stack parameters (for point sources only): exit gas velocity, stack diameter, exit gas temperature, and stack height.

Emissions data: for both criteria pollutants and chemical mechanism compounds (if file has been chemically speciated).

Each of the EPS3 modules reads a data record, processes the record, and then either (1) writes an updated data record to the output EMBR file, (2) writes an error record to the output error file, indicating the program was unable to process that record, or (3) determines that the record should be skipped.

Trailer Records

The trailer records contain the following information:

Number of data records contained in the EMBR file; and

For each EPS3 module that processed the data:
        number of input and output files,
        input file names,
        output file names,
        input emissions totals for criteria pollutants, and
        output emissions totals for criteria pollutants.

Essentially, the trailer section of an EMBR file contains a history of what processes were performed to create the file, including input/output filenames for each module and emissions totals. After processing all of the data records, the EPS3 module writes the trailer records from the input EMBR file trailer to the trailer of the output EMBR file and adds the information from the module being executed.

2.8   THE EMISSIONS MODEL ASCII RECORD (EMAR) FORMAT

The Emissions Model ASCII Record format, or EMAR, is an ASCII version of the binary EMBR format described in the previous section. The EPS3 provides the EMAR format to allow the user to read the data contained in the emissions file for quality control purposes. The EMBRET utility can be used to convert an entire EMBR file to the EMAR format (see Section 4 for a description of the EMBRET utility). The EMAR format is also used by most modules to

write the error file. This allows the user to inspect the data using an editor and determine if modifications are required.

Table 2-15 provides the EMAR file format. The fields in the EMAR and EMBR files are identical. Like the EMBR files, the EMAR files contain three types of records: header, data, and trailer. The information contained in these records is identical to that described above for EMBR files.

Table 2-15. Emissions Model ASCII Record (EMAR) file format.

Line	Variable	Columns	Type	Description
HEADER	*Header records are at the beginning of the file, preceding DATA records. The header records are more descriptive in the EMBRET output than in the output error files generated by the core modules.*			
1	FILTYP	1-30	C	File Type: POINTS AREA MOBILE FIREPTS SHIPS
2	RGUTME	1-10	R	Region origin UTM Easting (km)
	RGUTMN	11-20	R	Region origin UTM Northing (km)
	IRGZN	21-30	I	Region UTM zone
	NXRGN	31-40	I	Number of grid cells in east-west direction
	NYRGN	41-50	I	Number of grid cells in north-south direction
	DXRGN	51-60	R	Grid cell size (km) in east-west direction
	DYRGN	61-70	R	Grid cell size (km) in north-south direction
3	NCRTHD	1-10	I	Number of criteria pollutants
	NSPCHD	11-20	I	Number of speciated pollutants
4	CRTNAM( )	1-10	C	Criteria pollutant name
	ISAROAD( ) …	11-20	I	Corresponding pollutant code … for each NCRTHD criteria pollutant
5	SPCLST( )	1-10	C	Species name
	MOLWT( )	11-15	R	Molecular weight of species
	SPCRIT( ) …	17-21	I	Criteria pollutant generating the species … for each NSPCHD species
6+	PRGNM	1-30	C	Program name and version number
	EXDAT	31-40	C	Date program executed
	EXTIM	41-50	C	Time program executed
DATA	*The beginning of the data records section is indicated with the keyword indicator /DATA/.*			
D1+	FIP	1-5	C	FIPS state/county code
	SBRGN	7-11	C	Subregion code
	SICCD	13-16	C	Standard Industrial Classification code
	SCCCD	18-27	C	Source Category Code (ASC)
	RECTYP	29	C	Record Type. 'E' - elevated point 'L' - low level point 'M' - on-road mobile 'F' - fire source 'S' - shipping source ' ' - blank indicates area source
	PERIOD	31-32	C	Input inventory period type, e.g., PO
	INVBEG	34-41	I	Beginning Julian date/time (YYJJJHH)
	INVEND	43-50	I	End Julian date/time (YYJJJHH)
	IJCELL	52-57	I	Cell location of gridded inventory
	PLANT	59-68	C	NEDS plant identification code
	ISTACK	70-79	C	Stack number

Table 2-15. Emissions Model ASCII Record (EMAR) File Format. (concluded)

Line	Variable	Columns	Type	Description
	POINT	81-90	C	Point identification
	ISEGNO	92-94	I	Segment number
	UTME	96-105	R	UTM Easting coordinate (km) to define location of plant
	UTMN	107-116	R	UTM Northing coordinate (km) to define location of plant
	IUTMZN	118-119	I	UTM zone
	STKGEV	125-134	R	Stack exit gas velocity (m/s)
	STKDIA	136-145	R	Stack diameter (m)
	STKTMP	147-156	R	Stack exit gas temperature (K)
	STKHGT	158-167	R	Stack height (m)
	EMOUT(1)	169-178	R	Emissions (tons) of criteria pollutants
	EMOUT(2)	180-189	R	1 – NCRTHD. Format is (1X,E10.4) for each pollutant.
	… EMOUT(NCRTHD)	… *	R	
	SPCOUT(1)	*	R	Emissions (moles) of speciated pollutants
	SPCOUT(2)	*	R	1 – NSPCHD. Format is (1X,E10.4) for each pollutant.
	… SPCOUT(NSPCHD)	*	R	
TRAILER	*Trailer records are preceded by the keyword indicator /TRAILER/.*			
T1	NRECS	1-10	I	Number of DATA records in this EMAR file
T2**	PNAME	1-30	C	Program name and version
	NFIN	31-34	I	Number of input files for program PNAME
	NFOUT	35-38	I	Number of output files for program PNAME
T3+	FILIN()	1-60	C	NFIN input file names
T4+	FILOUT()	1-60	C	NFOUT output file names
T5	TOTIN	1-100	C	Criteria pollutant input totals to PNAME
T6	TOTOUT	1-100	C	Criteria pollutant output totals from PNAME

* The columns are determined by the number of pollutants in the file.
For criteria: the start column = 169 + ((criteria pollutant number-1)*11),
          end column = beginning column + 10
For speciated: the start column = 169 + ((NCRIT-1)*11 + (species number -1)*11.
           end column = beginning column + 10				

** Lines T2–T6 are repeated for each module which has processed the EMBR file.				

EPS3 modules that process EMBR files write input EMBR records that cannot be processed by the module to an error file in EMAR format. The entry modules PREPNT, PREAM, PREFIR, PRESHP and LBASE have ASCII input file formats, the error record output files for these modules are in the same format as the input data files. The user can review the data to determine what steps are necessary to include these records in the inventory. Like the EMBR file, all fields of the EMAR file will contain either a valid data value or a missing value flag. The missing value flag is a blank for a character field, a "-9" for an integer field, and a "-9.0" for a real field.

3. CORE MODULE DESCRIPTIONS

As discussed in Section 2.1, the core EPS3 system consists of FORTRAN modules. This section consists of detailed descriptions of each of those modules. Each description summarizes primary functions and provides an overview of the processing methodology of the module. Available user options for each module are discussed, and the selection of appropriate values for these options for a particular application is addressed. Input and output files are identified and described in detail.

The following list indicates the section in which each module is addressed:

   3.1   PREPNT (entry point for point source data)

   3.2   PREAM (entry point for county-level area, and mobile source data)

   3.3   LBASE (entry point for link-based emissions data)

   3.4   PREFIR (entry point for location specific fire data)

   3.5   PRESHP (entry point for shipping lane emissions data)

   3.6   CNTLEM (projection and control factor application)

   3.7   CHMSPL (chemical speciation)

   3.8   SPCEMS (chemical speciation)

   3.9   TMPRL (temporal allocation)

   3.10   PSTFIR (surface and elevated point specific fires)

   3.11   PSTSHP (surface and elevated shipping emissions)

   3.12   PSTPNT (elevated point source processing)

   3.13   PIGEMS (Plume-in-Grid processing)

   3.14   GRDEM (spatial allocation)

   3.15   MRGUAM (merge multiple CAMx emissions files)

As a quick reference for the user, Table 3-1 lists the input and output files for each of these EPS3 core modules.

Table 3-1. Input and output files for EPS3 core modules.

Module	Input files	Output files
PREPNT	USERIN: /PREPNT/, /CRITERIA POLLUTANT/, /DATE/, /REGION/, /COUNTY/, /CRITERIA TABLES/ AFS base inventory emissions file	PREPNT message file EMBR point source file stack report error records file (AFS format)
PREAM	USERIN: /CRITERIA POLLUTANT/, /DATE/, /REGION/, /COUNTY/, /CRITERIA TABLES/ AMS base inventory emissions file	PREAM message file EMBR area source file error records file (AMS format)
LBASE	USERIN: /LBASE/, /DATE/, /REGION/, /COUNTY/, /CRITERIA TABLES/ link based emissions file	LBASE message file EMBR motor vehicle file
PREFIR	USERIN: /PREFIR/, /FIRE BINS/, /CRITERIA POLLUTANT/, /DATE/, /REGION/, /COUNTY/, /CRITERIA TABLES/ Point specific fire emissions	PREFIR message file EMBR fire source file error records file
PRESHP	USERIN: /CRITERIA POLLUTANT/, /DATE/, /REGION/, /COUNTY/, /CRITERIA TABLES/ Shipping lane shipping emisisions	PRESHP message file EMBR fire source file error records file
CNTLEM	USERIN: /CNTLEM/, /COUNTY/, /CRITERIA TABLES/, /SPECIES TABLES/ control factors file: /PROJECT PTS/, /PROJECT AMS/, /SOURCE CATEGORY/, /FIPS CODE/ EMBR file	CNTLEM message file EMBR file
SPCEMS	USERIN: /SPCEMS/, /SPECIES LIST/, /COUNTY/, /CRITERIA TABLES/, /SPECIES TABLES/ SCC(ASC)/speciation profiles cross reference by criteria speciation factors conversion factors *(optional)* EMBR file	SPCEMS message file EMBR file EMAR error records file
CHMSPL	USERIN: /CHMSPL/, /DEFAULT SPLITS/, /SPECIES LIST/, /COUNTY/, /CRITERIA TABLES/, /SPECIES TABLES/ SCC(ASC)/speciation profiles cross reference chemical mechanism compound split factors EMBR file	CHMSPL message file EMBR file EMAR error records file
TMPRL	USERIN: /TMPRL/, /DATE/, /COUNTY/, /CRITERIA TABLES/, /SPECIES TABLES/ SCC(ASC)/temporal profiles cross reference temporal profiles EMBR file	TMPRL message file EMBR file EMAR error records file
PSTFIR	USERIN: /LAYERS/, /FIRE BINS/, /DATE/, /REGION/, /COUNTY/, /SPECIES LIST/, /CRITERIA TABLES/, /SPECIES TABLES/ EMBR fire source file	PSTFIR message file CAMx low level emissions file Stack list file (optional) Stack emissions data file (optional) EMAR error records file
PSTSHP	USERIN: /LAYERS/, /DATE/, /REGION/, /COUNTY/, /SPECIES LIST/, /CRITERIA TABLES/, /SPECIES TABLES/ SCC/Vessel cross reference EMBR shipping source file	PSTSHP message file CAMx low level emissions file Stack list file Stack emissions data file EMAR error records file

Table 3-1. Input and output files for EPS3 core modules (concluded).

Module	Input files	Output files
PSTPNT	USERIN: /DATE/, /REGION/, /COUNTY/, /SPECIES LIST/, /CRITERIA TABLES/, /SPECIES TABLES/ EMBR point source file	PSTPNT message file Stack list file Stack emissions data file EMAR error records file
PIGEMS	USERIN: /DATE/, /REGION/, /COUNTY/, /CRITERIA POLLUTANT/, /SPECIES LIST/, /CRITERIA TABLES/, /SPECIES TABLES/, /THRESHOLD VALUE/, /THRESHOLD MAP/, /COMBINE STACKS/ Master stack file Stack list(s) from PSTPNT Stack emissions file(s) from PSTPNT	PIGEMS message file merged master stack file with sources flagged as PiGs CAMx elevated point source emissions file
GRDEM	USERIN: /GRDEM/,/DATE/, /REGION/, /COUNTY/, /SPECIES LIST/, /CRITERIA TABLES/, /SPECIES TABLES/ SCC(ASC)/spatial surrogate cross reference (optional) gridded spatial surrogates (optional) link data *(optional)* EMBR file	GRDEM message file EMBR *or* CAMx low level emissions file EMAR error records file gridded surrogate report (optional)
MRGUAM	USERIN: /MRGUAM/ *(optional)*, /DATE/, /REGION/, /SPECIES LIST/, /CRITERIA TABLES/, /SPECIES TABLES/ UAM low level emissions files	MRGUAM message file merged CAMx low level emissions file

3.1 PREPNT

The PREPNT (**PRE**processor for **PoiNT** source emissions) module is the entry point to EPS3 for point source emissions data. The primary functions of PREPNT are

   Identification of sources within the modeling domain,

   Initial screening of which sources are to be treated as elevated point sources, and

   Reformat the input AFS emissions inventory into EMBR format.

PREPNT reads point source data from the AFS work file (see Table 3-2), including stack parameters, process and geographical identification codes, pollutant code and corresponding emission rate. The AFS work file may include any criteria pollutant codes specified in the /CRITERA POLLUTANT/ packet of the USERIN. Although the format of the input AIRS AFS work file permits emissions to be specified as yearly, seasonal, typical day, or day-specific, PREPNT converts the emissions to an internal format of average daily rate. The units of the emissions values in the AFS work file depends on the period type specified on the AFS record. For an annual period type, the emission units are tons per year. For the peak ozone and peak CO period types, the units are tons per typical weekday. This means that the emission rate for a peak ozone or peak CO period type represents the emissions on a weekday during the season. The rate will only be adjusted by the temporal allocation module, TMPRL when processing a weekend episode day. For the average day period type, the units are tons per average day. In this case, the daily emissions may be adjusted by the TMPRL module when processing any day of the week. Units for the specific interval period type are tons per specified period. That is, if the specified

interval is just one hour, the units are tons per hour. If the specified interval consists of the entire month of June, the units are tons per month.

For AFS work files containing annual emissions, PREPNT divides the annual emissions rate (ton/year) by 365 days per year to generate an annual average daily emissions rate. Exhibit 3-1 shows a portion of an AFS file for annual emissions. For AFS work files containing seasonal (or other specified interval) emissions, PREPNT divides the emissions rate for the interval (tons per interval period) by the number of days in the interval to calculate the average daily emissions rate. For AFS work files containing typical season day or average day emission rates, no adjustment is performed.

EMBR records that contain a source identified as an elevated source will be further processed by the PSTPNT and PiGEMS modules. Those sources identified as low-level will be processed by the module, GRDEM, to generate an emissions file for input to the CAM$_X$.

Table 3-2. AIRS Facility Subsystem (AFS) data input into the PREPNT module and TMPFAC utility.

Line	Variable	Columns	Type	Description
1+	ITYPE	1	C	Inventory TYPE (ignored) A = Adjusted B = Base R = RFP M = Modeling
	IREFYR	3-4	I	Projection year (optional)
	IBASYR	6-7	I	Inventory base year (optional)
	INETYP	9-10	C	Emissions Type (ignored) AC = Actual AA = Allowable based on activity level limit AB = Allowable based on both activity level and emission factor limits AE = Allowable based on emissions total AF = Allowable based on emission factor limit GB = Growth and Base Controls GN = Growth and New Controls LB = Limit and Base Controls LN = Limit and New Controls
	INFIPS	12-16	C	FIPS state/county code
	INSBRG	18-22	C	Subregion code (city FIPS) (optional)
	INSIC	24-27	C	Standard Industrial Classification code (SIC)
	INSCC	29-38	C	Source Classification Code (SCC)
	INPLNT	40-49	C	Plant identification code
	INSTCK	51-60	C	Stack identification code
	INPNT	62-71	C	Emission point identifier (optional)
	INSEG	73-75	C	Segment identification code (optional)
	IPEROD	77-78	C	Period Type Blank = Annual PO = Peak O$_3$ typical weekday PC = Peak CO typical weekday AD = Average Day S = Specified interval

Table 3-2. AIRS Facility Subsystem (AFS) data input into the PREPNT module and TMPFAC utility (concluded).

Line	Variable	Columns	Type	Description
	IBEGDT	80-87	I	Beginning period interval date/time; time is in military format (YYMMDDHH)
	IENDDT	89-96	I	Ending period interval date/time; time is in military format (YYMMDDHH). Note: the time interval stops at the <u>start</u> of the specified end hour.
	XLOC	98-107	R	Latitude (decimal degrees) or Easting coordinate (km) to define location of plant
	YLOC	109-118	R	Longitude (decimal degrees) or Northing coordinate (km) to define location of plant
	IZONE	120-121	I	UTM zone associated with UTM coordinates given for a plant (optional if location is lat/lon)
	STKHT	123-127	R	Stack height (m)
	STDIAM	129-133	R	Stack diameter (m)
	STEXTP	135-139	R	Stack exit gas Temperature (°K)
	STEXVL	141-145	R	Stack exit gas Velocity (m/s)
	INTHRU(4)	147-149 151-153 155-157 159-161	I	Annual throughput (%) for the periods: (optional) December - February March - May June - August September - November
	IHRPDY	163-164	I	Hours per day operating (optional)
	IBEGHR	166-167	I	Starting hour (optional) 0 = hour 0-1 23 = hour 23-24
	IDYPWK	168-169	I	Days per week operating (optional)
	IHRPYR	171-174	I	Hours per year operating (optional)
	INPOL	176-180	I	Pollutant code
	CRTPOL	182-191	R	Emissions of specified pollutant Units depend on the Period Type Annual = tons/year PO/PC = tons/typical weekday AD = tons/average day S = tons/period (the period is specified using the beginning and ending time fields)
	PLNTNM	220-260	C	Plant name (optional)

```
B 99 99 AC 48001      4922  20200202        0012          1        005     PO 99060100 99083124   381.0670  -873.7402  0  16.8  0.46
686   49.8  24   24   28   24 24    7  168 42101   0.030000                        TEXAS UTILITIES FUEL COMPANY

B 99 99 AC 48001      4922  20200202        0012          1        005     PO 99060100 99083124   381.0670  -873.7402  0  16.8  0.46
686   49.8  24   24   28   24 24    7  168 42603   0.020000                        TEXAS UTILITIES FUEL COMPANY

B 99 99 AC 48001      4922  20200202        0012          1        005     PO 99060100 99083124   381.0670  -873.7402  0  16.8  0.46
686   49.8  24   24   28   24 24    7  168 43104   0.010000                        TEXAS UTILITIES FUEL COMPANY

B 99 99 AC 48001      4922  20200202        0012          1        006     PO 99060100 99083124   381.0670  -873.7402  0  16.8  0.46
686   49.8  24   24   28   24 24    7  168 42101   0.030000                        TEXAS UTILITIES FUEL COMPANY

B 99 99 AC 48001      4922  20200202        0012          1        006     PO 99060100 99083124   381.0670  -873.7402  0  16.8  0.46
686   49.8  24   24   28   24 24    7  168 42603   0.020000                        TEXAS UTILITIES FUEL COMPANY

B 99 99 AC 48001      4922  20200202        0012          1        006     PO 99060100 99083124   381.0670  -873.7402  0  16.8  0.46
686   49.8  24   24   28   24 24    7  168 43104   0.010000                        TEXAS UTILITIES FUEL COMPANY

B 99 99 AC 48001      4922  20200202        0012          1        007     PO 99060100 99083124   381.0670  -873.7402  0  16.8  0.76
620    7.1  24   24   28   24 24    7  168 42101   0.020000                        TEXAS UTILITIES FUEL COMPANY

B 99 99 AC 48001      4922  20200202        0012          1        007     PO 99060100 99083124   381.0670  -873.7402  0  16.8  0.76
620    7.1  24   24   28   24 24    7  168 42603   0.060000                        TEXAS UTILITIES FUEL COMPANY

B 99 99 AC 48001      4922  20200202        0012          1        007     PO 99060100 99083124   381.0670  -873.7402  0  16.8  0.76
620    7.1  24   24   28   24 24    7  168 43104   0.010000                        TEXAS UTILITIES FUEL COMPANY

B 99 99 AC 48001      4922  20200202        0012          1        008     PO 99060100 99083124   381.0670  -873.7402  0  16.8  0.76
620    7.1  24   24   28   24 24    7  168 42101   0.020000                        TEXAS UTILITIES FUEL COMPANY

B 99 99 AC 48001      4922  20200202        0012          1        008     PO 99060100 99083124   381.0670  -873.7402  0  16.8  0.76
620    7.1  24   24   28   24 24    7  168 42603   0.060000                        TEXAS UTILITIES FUEL COMPANY

B 99 99 AC 48001      3296  30501213        0013          1        006     PO 99060100 99083124   406.6810  -879.0225  0  22.6  0.98
700   11.0  25   25   25   25 24    7  168 43104   0.010000                        OWEN CORNING

B 99 99 AC 48001      3296  30501208        0013          1        008     PO 99060100 99083124   406.6810  -879.0225  0   0.3  0.08
811   14.2  25   25   25   25 24    7  168 11101   0.100000                        OWEN CORNING

B 99 99 AC 48001      3296  30501208        0013          1        008     PO 99060100 99083124   406.6810  -879.0225  0   0.3  0.08
811   14.2  25   25   25   25 24    7  168 81102   0.120000                        OWEN CORNING

B 99 99 AC 48001      3296  30501208        0013          1        008     PO 99060100 99083124   406.6810  -879.0225  0   0.3  0.08
811   14.2  25   25   25   25 24    7  168 42101   0.020000                        OWEN CORNING

B 99 99 AC 48001      3296  30501208        0013          1        008     PO 99060100 99083124   406.6810  -879.0225  0   0.3  0.08
811   14.2  25   25   25   25 24    7  168 42603   0.010000                        OWEN CORNING.
```

Exhibit 3-1. Example of AFS file input to PREPNT.

> ➢ **Special Note**
> PREPNT will consolidate multiple emission records which are from a single
> release point if the data are arranged consecutively in the AFS input file.
> Prior to running PREPNT, the AFS data should be sorted using the
> following UNIX sort command:
> :
> sort -o *<SORTED_OUTPUT_FILE>* \
> -t^ +0.12 -0.16 +0.40 -0.49 +0.51 \
>   -0.60 +0.62 -0.71 +0.29 -0.38 +0.176 -0.180   *<INPUT_FILE>*
>
> This step will result in a smaller EMBR output file and efficient execution of
> subsequent EPS3 modules and utilities.

Elevated Source Screening

PREPNT screens the input data to determine which point source emissions records will be treated as elevated sources. This determination is based on the final plume height as calculated by the Briggs effective height algorithm using default meteorological parameters representing stable conditions.

> ➢ **Processing Note**
> The meteorological parameters used by PREPNT to determine effective
> plume height have been selected with the goal of ensuring that any sources
> with emissions that might possibly enter the upper layers of the modeling
> grid will be treated as elevated sources. These parameters, which are
> hardcoded into the PREPNT module, are as follows:
>
> | | |
> |---|---|
> | Pasquill stability | Class B |
> | Wind speed | 2 m/s |
> | Vertical ambient temperature gradient | 0 K/m |
> | Potential temperature lapse rate | 0.02 K/m |
> | Downwind distance at which turbulence begins to dominate | 0 m |
> | Ambient temperature | 293 K |
> | Ambient barometric pressure | 960 mb |

If the calculated plume height of a source is above the user-supplied cutoff value, the emissions record is flagged with the letter "E", which indicates an elevated source; otherwise the record is flagged with the letter "L", meaning "low level". When determining an appropriate plume height cutoff, the user should consult with the CAM_X modeler; the cutoff value will usually be selected based on considerations of both minimum episodic mixing heights and the computing requirements for elevated source treatment. If the specified cutoff is too high, emissions from

some sources may not be allocated to the correct vertical layers of the modeling grid. Conversely, if the specified cutoff is lower than warranted, sources whose emissions never leave the lowest vertical layer of the model may unnecessarily be treated as elevated, thus increasing the computational time required by the CAM_X without significantly increasing the accuracy of the CAM_X-predicted concentrations.

Data Validity Screening

Since PREPNT is one of the entry points to EPS3, the PREPNT module performs various data validity checks to prevent further processing of erroneous data. The FIPS state/county identification codes are checked against the user-supplied county list (specified in the /COUNTY/packet of the USERIN) to ensure that the correct region is included in the AFS file. A message is written to the message output file indicating which counties in the county list had no corresponding AFS records. In addition, each of the stack parameters on the point source record undergo a "reasonableness" check; erroneous records are processed in one of two ways based on the "process missing stack" option specified in the /PREPNT/ packet of the USERIN. If the option is set to "YES", PREPNT replaces the invalid stack parameter value with the user-supplied default value and continues processing. If this option is set to "NO", the record is not processed (i.e., not written to EMBR), but rather is written to a separate error file (this file may be empty if none of the data extracted from the AFS falls outside of the specified "reasonable" range).

> ➢ **Processing Note**
> The default stack parameters provided with EPS3 in the /PREPNT/ packet of the USERIN file have been selected to ensure that emissions from sources missing stack parameters remain in the lowest vertical layer of the modeling grid. The default values are
>
> | | |
> |---|---|
> | Stack height | 3 m |
> | Stack diameter | 0.2 m |
> | Gas temperature | 294 K |
> | Gas exit velocity | 0.5 m/s |

Input Files

PREPNT requires two input files: the user input file USERIN and the AFS work file. PREPNT reads the following seven packets from USERIN.

/PREPNT/   The /PREPNT/ packet contains the input parameters unique to the PREPNT program; the packet also includes the default values for the stack height, stack diameter, stack temperature, exit velocity, and the plume height cutoff value (Table 3-3). This includes the user options for input coordinates in either geodesic or UTM coordinates and for processing missing stack parameters. (Exhibit 3-2)

ENVIRON

> ➢ **Special Note**
> PREPNT manipulates the input geographical coordinates based on the coordinate flag in the /PREPNT/ packet. The user must ensure the location information is in the same coordinate system used for the modeling application. The primary coordinate forms are geodesic, UTM and Lambert Conformal Projection (LCP). When using the LCP system, standard practice is to convert the AFS coordinates outside of EPS3 and set the "Convert Coordinates" flag to "NO".

```
/PREPNT/
Convert Coordinates: NO
Process Missing stk: YES
Plume ht Cutoff (M): 50.0
Default stk ht (M) : 3.0
Default diam (M)    : 0.2
Default temp (K)    : 294.
Default veloc (M/S): 0.5
/END/
```

Exhibit 3-2. PREPNT packet of USERIN.

Table 3-3. /PREPNT/ packet of EPS3 global user input file, USERIN.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	C	Packet identifier - /PREPNT/
2		1-20		Not used
	LGEODS	21-30	C	Flag which determines if input coordinates are to be converted: YES = input coordinates are geodesic and should be converted NO = input coordinates match modeling domain and should not be converted
3		1-20		Not used
	LPRCES	21-30	C	Flag which determines if missing stack parameters are replaced with default values: YES = replace with defaults and process NO = write record to error file and skip
4		1-20		Not used
	PCUTOF	21-30	R	Plume height cutoff for elevated points (meters)
5		1-20		Not used
	DFHITE	21-30	R	Default stack height (meters)
6		1-20		Not used
	DFDIAM	21-30	R	Default stack diameter (meters)
7		1-20		Not used
	DFTEMP	21-30	R	Default stack gas temperature (°K)
8		1-20		Not used
	DFVEL	21-30	R	Default stack gas exit velocity (m/s)
9	KEYEND	1-20	A	Packet terminator - /END/

/CRITERIA POLLUTANT/ PREPNT reads this packet (Table 2-9) to determine which of the input pollutants to include in the modeling inventory. The criteria pollutants will be stored on the EMBR record in the same order they appear in the packet.

/DATE/   PREPNT reads the /DATE/ packet (Table 2-6) to obtain the date of the modeling episode. For period-specific input AFS work files, PREPNT checks that the month and day of the modeling episode corresponds to the time period specified on each input AFS record.

/REGION/   This packet contains the definition of the modeling domain (Table 2-7) and allows PREPNT to exclude those point sources located outside of the modeling region, thus reducing the computer processing time required by subsequent modules.

/COUNTY/ This packet contains the list of counties within the modeling domain (Table 2-8). PREPNT reads this packet to check the county identification code specified on each input record against the region county list, and to determine if any counties from the region list had no corresponding AFS data records, i.e., identify possible missing input emission data. The /COUNTY/ packet also contains county time zone designation.

/CRITERIA TABLES/ This packet specifies which output tables, if any, the user wants to include in the output message file (Table 2-11). See Section 2.4 for a full discussion on the output tables. Since the emissions input to PREPNT are not typically speciated, the /SPECIES TABLES/ packet is not read.

The second input file is the point source emissions file, which is in the AFS work file format (Table 3-2).

Output Files

The PREPNT program produces four output files: the PREPNT message file, an EMBR file, a stack report file, and an error file containing input records that PREPNT was unable to process due to errors.

The first section of the PREPNT message file summarizes input and output file names, episode and region definition parameters, and the default stack parameters specified by the user. This section is followed by a summary of the number of records processed, the domain-wide criteria pollutant emissions totals for the input and output files, and warning messages indicating counties in the /COUNTY/ packet of USERIN for which no records were found in the AFS work file. The final section of the PREPNT message file consists of summary tables selected by the user in the /CRITERIA TABLES/ packet of USERIN.

The second output file is the point source emissions inventory EMBR file, with a specified file type of "POINTS" in the header records.

The third PREPNT output file, called the stack report file, summarizes stack and emissions data for each source written to the output EMBR file. For each source within the modeling domain, this file lists geographical, facility and stack identification codes, source location, stack parameters (with an indication of whether stack data were obtained from the AFS work file or

from the user-specified defaults), the effective plume height calculated by PREPNT and emission values. The stack report file also indicates which sources will be treated as elevated sources with an asterisk in column one. A sample stack report file is shown in Exhibit 3-4.

A fourth output file, which may be empty, contains the input AFS records which have insufficient data for processing. This file is written in the AFS work file format to facilitate review, correction, and reprocessing.

Exhibit 3-3 shows a sample of a PREPNT job script.

```
#!/bin/csh
#
#    --- Sample job script for running the
#        EPS3 module PREPNT
#
set EXEC = /models/eps3/src
#
set SCENARIO = test_problem
#
# --- sort the AFS file ---
#
sort -o ../inputs/AFS.points.$SCENARIO \
-t^ +0.12 -0.16 +0.40 -0.49 +0.51 \
   -0.60 +0.62 -0.71 +0.29 -0.38 +0.176 -0.180 \
                        ../inputs/AFS.points.$SCENARIO
#
#
rm -f ../msg/msg.prepnt.$SCENARIO
rm -f ../embr/embr.prepnt.$SCENARIO
rm -f ../reports/stkrpt.prepnt.$SCENARIO
rm -f ../error/error.prepnt.$SCENARIO
#
echo "----------------------------------------------"
echo "    Running PREPNT for $SCENARIO"
echo "----------------------------------------------"
#
$EXEC/prepnt/prepnt << IEOF
USERIN file        :../inputs/userin.$SCENARIO
Input AFS file     :../inputs/AFS.points.$SCENARIO
Output Messages    :../msg/msg.prepnt.$SCENARIO
Output EMBR        :../embr/embr.prepnt.$SCENARIO
Stack Report       :../reports/stkrpt.prepnt.$SCENARIO
EMAR error file    :../error/error.prepnt.$SCENARIO
IEOF
```

Exhibit 3-3. Example of a PREPNT job script.

```
                          Stack parameters and emissions
                          Emissions reported for average day
   NOTE: Negative numbers indicate defaults were used.
   NOTE: A * indicates stacks treated as elevated point sources.

    FIPS  Plant    Stack        UTM      UTM    Stack  Stack   Exit   Exit  Plume
    Code  ID       ID           East     North  Height Diam    Temp   Veloc height    NOX      CO       VOC
                                (km)     (km)   (m)    (m)     K      (m/s) (m)        tons     tons     tons
   -----------------------------------------------------------------------------------------------------------
   * 48001 0012     1           381.067  -873.740  16.80  0.46  686.0  49.80   97.6    0.040    0.060    0.020
   * 48001 0012     1           381.067  -873.740  16.80  0.76  620.0   7.10   54.2    0.120    0.040    0.020
     48001 0012     1           381.067  -873.740   0.90  1.34  298.0  15.10   12.5    0.       0.       0.050
   * 48001 0013     1           406.681  -879.023  22.60  0.98  700.0  11.00  104.5    0.130    0.       0.010
     48001 0013     1           406.681  -879.023   0.30  0.08  811.0  14.20    2.8    0.010    0.020    0.080
   * 48001 0013     1           406.681  -879.023  22.60  1.01  478.0  15.20  103.1    0.010    0.060    0.010
     48001 0020     1           425.838  -869.119   8.50  0.91  294.0  -0.50    8.7    0.       0.       0.720
   * 48005 0001     1           508.081  -933.727  22.90  2.26  339.0  10.10  113.2    0.180    1.610    0.030
   * 48005 0001     1           508.081  -933.727  21.30  0.70  450.0  14.30   62.3    0.       0.       1.030

   * 48005 0001     1           508.081  -933.727  21.30  1.58  319.0   9.60   56.0    0.       0.       0.200
     48005 0001     1           508.081  -933.727   5.50  0.93  298.0   9.00   10.1    0.       0.       0.110
   * 48005 0002     1           508.081  -933.727  22.60  0.97  355.0  14.90   63.7    0.       0.020    0.110
   * 48005 0002     1           508.081  -933.727  20.10  0.80  355.0  15.90   52.4    0.       0.020    0.090
   * 48005 0002     1           508.081  -933.727  25.90  0.88  332.0  25.70   65.6    0.       0.       0.020
   * 48005 0002     1           508.081  -933.727  36.60  1.97  341.0  17.80  152.2    0.670    2.690    0.080
   * 48005 0002     1           508.081  -933.727  15.20  1.80  333.0   6.80   58.7    0.200    2.080    0.
       .
       .
       .
     48505 0005     1            64.142 -1408.027   3.00  0.09  700.0  42.10    9.2    0.040    0.010    0.
     48505 0005     1            64.142 -1408.027   4.00  0.19  863.0  89.30   41.0    0.100    0.200    0.020
   * 48505 0005     1            64.142 -1408.027   5.80  0.41  658.0  78.60   99.3    0.080    0.140    0.010
   -----------------------------------------------------------------------------------------------------------
   NOTE: Negative numbers indicate defaults were used.
   NOTE: A * indicates stacks treated as elevated point sources.
```

Exhibit 3-4. Example of a stack report file created by PREPNT.

3.2 PREAM

The PREAM (**PRE**processor for **A**rea and **M**obile sources) module serves as the entry point to EPS3 for area and non-link based mobile source emissions data. The primary function of the PREAM module is

> Reformat an emission inventory from the AIRS Area and Mobile Subsystem (AMS) format into the EMBR format.

The format of the input AMS work file permits emissions to be specified as either annual or typical day emissions for a specified period of any criteria pollutant codes specified in the /CRITERIA POLLUTANT/ packet of the USERIN. PREAM reads the AMS work file, converts the emissions to an average daily rate for the time period of the AMS work file, and writes the output records to the EMBR file. The units of the emissions values in the AMS work file depends on the period type specified on the AMS record. For an annual period type, the emission units are tons per year. For the peak ozone and peak CO period types, the units are tons per typical weekday. This means that the emission rate for a peak ozone or peak CO period type represents the emissions on a weekday during the season. The rate will only be adjusted by the temporal allocation module, TMPRL, when processing a weekend episode day. For the average day period type, the units are tons per average day. In this case, the daily emissions may be adjusted by the TMPRL module when processing any day of the week. Units for the specific interval period type are tons per specified period. That is, if the specified interval is just one hour, the units are tons per hour. If the specified interval consists of the entire month of June, the units are tons per month.

PREAM converts emissions to an average daily rate in the following manner. For AMS work files containing annual emissions, PREAM divides the annual emissions rate (tons per year) by 365 days to generate an annual average daily emissions rate. For AMS work files containing a specified emissions interval, PREAM calculates the average daily emissions by dividing the emissions rate for the interval (tons per interval period) by the number of days in the interval. For AMS work files containing typical season day, average day, or hourly emission rates, PREAM does not adjust the emissions rates.

> ➢ **Special Note**
> PREAM will consolidate multiple emission records which are from a single source category within a county, if the data are arranged consecutively in the AMS input file. Prior to running PREAM, the AMS data should be sorted using the following UNIX sort command:
> :
> sort -o *<SORTED_OUTPUT_FILE>* *<INPUT_FILE>*
>
> This step will result in a smaller EMBR output file and efficient execution of subsequent EPS3 modules and utilities.

Data Validity Screening

PREAM is an entry module for the EPS3 system. Accordingly, the PREAM module performs some initial screening of the input AMS work file to identify inconsistencies between the data contained in the AMS file and user-specified parameters. PREAM checks the state/county identification code on each input record against the user-supplied county list in the /COUNTY/ packet of the USERIN file to ensure that the correct region is included in the AMS file. At program completion, PREAM writes a series of warning messages to the message output file indicating which counties in the county list had no corresponding AMS records.

Input Files

The PREAM module requires four input files. The first input file is the USERIN file, from which PREAM reads five packets:

/CRITERIA POLLUTANT/ PREAM reads this packet (Table 2-9) to determine which of the input pollutants to include in the modeling inventory. The criteria pollutants will be stored on the EMBR record in the same order they appear in the packet.

/DATE/   PREAM reads the /DATE/ packet (Table 2-6) to obtain the date of the modeling episode. For period-specific input AMS work files, PREAM checks that the month and day of the modeling episode corresponds to the time period specified on each input AMS record.

/REGION/   This packet contains the definition of the modeling domain (Table 2-7) and allows PREAM to exclude those sources located outside of the modeling region, thus reducing the computer processing time required by subsequent modules.

/COUNTY/ This packet contains the list of counties within the modeling domain (Table 2-8). PREAM reads this packet to check the county identification code specified on each input record against the region county list, and to determine if any counties from the region list had no corresponding AMS data records, i.e., identify possible missing input emission data. The /COUNTY/ packet also contains county time zone designation.

/CRITERIA TABLES/ This packet specifies which output tables, if any, the user wants to include in the output message file (Table 2-11). See Section 2.4 for a full discussion on the output tables. Since the emissions input to PREAM are not typically speciated, the /SPECIES TABLES/ packet is not read.

The second input file is the AMS work file for area and mobile source emissions (Table 3-4). A sample AMS work file is shown in Exhibit 3-5.

Table 3-4. AIRS Area and Mobile Source (AMS) data input into the PREAM module.

Line	Variable	Columns	Type	Description
1+	ITYPE	1	C	Inventory type (optional) A = Adjusted B = Base R = RFP M = Modeling
	IREFYR	2-3	I	Projection year (optional)
	IBASYR	5-6	I	Inventory base year (optional)
	INETYP	7-8	C	Emissions Type AA = Allowable based on activity level limit AB = Allowable based on both activity level and emission factor limits AC = Actual AD = Average day AE = Allowable based on emissions limit AF = Allowable based on emission factor limit GB = Growth and Base Controls GN = Growth and New Controls LB = Limit and Base Controls LN = Limit and New Controls
	INFIPS	9-13	C	FIPS state/county code
	INSBRG	15-19	C	Subregion code (city FIPS) (optional)
	INSIC	21-24	C	Standard Industrial Classification code (optional)
	INASC	26-35	C	Area Source Category (ASC)

	IPEROD	37-38	C	Period Type
				Blank = annual
				  PO = Peak O$_3$ typical weekday
				  PC = Peak CO typical weekday
				  AD = Average Day
				  S = Specified interval

	IBEGDT	40-47	I	Beginning period interval date/time; time is in military format (YYMMDDHH)
	IENDDT	49-56	I	Ending period interval date/time; time is in military format (YYMMDDHH). Note: the time interval stops at the <u>start</u> of the specified end hour.
	INPOL	58-62	I	Pollutant code

	CRTPOL	64-73	R	Emissions of specified pollutant
				Units depend on the Period Type
				Annual = tons/year
				PO/PC = tons/typical weekday
				  AD = tons/average day
				  S = tons/period (the period is specified using the beginning and ending time fields)

```
 B99    AC48001              2102005000 PO 99060100 99083124 42603    0.010000
 B99    AC48001              2102007000 PO 99060100 99083124 42101    0.000400
 B99    AC48001              2103006000 PO 99060100 99083124 42101    0.022500
 B99    AC48001              2103006000 PO 99060100 99083124 42603    0.026800
 B99    AC48001              2103006000 PO 99060100 99083124 43104    0.001500
 B99    AC48001              2103007000 PO 99060100 99083124 42603    0.000300
 B99    AC48001              2104006000 PO 99060100 99083124 42101    0.006000
 B99    AC48001              2104006000 PO 99060100 99083124 42603    0.014000
 B99    AC48001              2104006000 PO 99060100 99083124 43104    0.000800
 B99    AC48001              2104007000 PO 99060100 99083124 42603    0.010000
 B99    AC48001              2310000000 PO 99060100 99083124 42101    0.542700
 B99    AC48001              2310000000 PO 99060100 99083124 42603    0.870500
 B99    AC48001              2310000000 PO 99060100 99083124 43104    3.286300
 B99    AC48001              2401001001 PO 99060100 99083124 43104    0.024400
 B99    AC48001              2401001005 PO 99060100 99083124 43104    0.027600
 B99    AC48001              2401001006 PO 99060100 99083124 43104    0.009200
 B99    AC48001              2401001010 PO 99060100 99083124 43104    0.019600
 B99    AC48001              2401001011 PO 99060100 99083124 43104    0.015500
 B99    AC48001              2401001015 PO 99060100 99083124 43104    0.030200
 B99    AC48001              2401001020 PO 99060100 99083124 43104    0.011100
 B99    AC48001              2401001025 PO 99060100 99083124 43104    0.009000
 B99    AC48001              2401001050 PO 99060100 99083124 43104    0.060000
 B99    AC48001              2401001060 PO 99060100 99083124 43104    0.032800
 B99    AC48001              2401005500 PO 99060100 99083124 43104    0.000400
 B99    AC48001              2401005600 PO 99060100 99083124 43104    0.007700
 B99    AC48001              2401005700 PO 99060100 99083124 43104    0.012000
 B99    AC48001              2401005800 PO 99060100 99083124 43104    0.001700
 B99    AC48001              2401008000 PO 99060100 99083124 43104    0.020800
 B99    AC48001              2401015000 PO 99060100 99083124 43104    0.003100
 B99    AC48001              2401030000 PO 99060100 99083124 43104    0.019800
 B99    AC48001              2401055000 PO 99060100 99083124 43104    0.007600
 B99    AC48001              2415105000 PO 99060100 99083124 43104    0.010000
```

Exhibit 3-5. Example of an AMS file used as input to PREAM.

Output Files

The PREAM program produces three output files: a message file, an EMBR file, and an error file.

The first section of the message output file summarizes the input and output file names and provides information regarding the input AMS work file and user-defined modeling region. The next section summarizes domain-wide input and output emissions totals and totaled processed emission outputs for criteria pollutants and lists any counties specified in the /COUNTY/ packet of the USERIN file for which no emissions records were found in the AMS work file. The final section of the message output file includes summary tables selected in the USERIN /CRITERIA TABLES/ packet. Note that at this point in processing the emissions totals are for an entire county, not just those areas actually located within the modeling domain. Thus, the output emissions totals may include emissions for portions of counties not in the modeling domain. Exhibit 3-6 shows a sample of a PREAM message file.

PREAM creates an EMBR file containing emissions records for the sources included in the AMS file. These sources may include area sources, off-road vehicle, on-road vehicle, or other general sources.

The third output file will contain data only if PREAM encounters records with insufficient data for processing. PREAM writes these records to a separate file in the AMS work file format to facilitate reprocessing of the data once corrections have been made.

Exhibit 3-7 shows a sample PREAM job script.

```
                EPS3 PREAM module v. 1.00 Aug 2004

         Input Files
         USERIN file                  :../inputs/userin.regional.othr.wkd
         Input AMS file               :../data/ams.TX_99.area_base1_srt

         Output Files
         Output EMBR file             :../embr/embr.pream.ar.tx_99tceq
         EMAR error file              :../error/error.pream.ar.tx_99tceq


                EPS3 PREAM module v. 1.00 Aug 2004

         Input Files
         USERIN file                  :../inputs/userin.test_problem
         Input AMS file               :../inputs/AMS.area.test_problem

         Output Files
         Output EMBR file             :../embr/embr.pream.test_problem
         EMAR error file              :../error/error.pream.test_problem


                EPS3 PREAM module v. 1.00 Aug 2004       07/25/07 18:41:31

         File note                    :CAMx Modeling of Tx regional, 9/13/99
         Episode date (Calander)      :990913
         Episode date (Julian)        :99256
         Beginning hour               :    0
         Ending hour                  :   24
         Number of counties           :  213

 Number of input records read:    15443
 Number of output EMBR records written:    15443
 Number of input records written to EMAR:      0
 Number of records skipped:         0

 Total Emissions Processed
                   English Tons/Day
                      NOX          CO         VOC
 -----------------------------------------------------------
 Input Emissions      647.1180   1006.4943   1826.7257
 Output Emissions     647.1180   1006.4943   1826.7257
 Emissions Skipped       0.          0.          0.
 Written to Err File     0.          0.          0.
 -----------------------------------------------------------

                   Criteria Pollutant Emissions by County
                          English Tons/Day

  County    Input     Output    Input     Output    Input     Output
            NOX       NOX       CO        CO        VOC       VOC
 --------------------------------------------------------------------------
   48001    0.9765    0.9765    1.9839    1.9839    7.0344    7.0344
   48005    0.2381    0.2381    1.9036    1.9036    6.4124    6.4124
   48007    0.7783    0.7783    4.7766    4.7766    1.9559    1.9559
   48009    0.1590    0.1590    1.9377    1.9377   19.9558   19.9558
   48011    0.2025    0.2025    2.6541    2.6541    1.1957    1.1957
```

Exhibit 3-6. Example of a PREAM message file.

ENVIRON

```
#!/bin/csh
#
#   --- Sample job script for running the
#       EPS3 module PREAM
#
set EXEC = /models/eps3/src
#
set SCENARIO = test_problem
#
# --- sort the AMS file ---
#
sort -o ../inputs/AMS.area.$SCENARIO \
                          ../inputs/AMS.area.$SCENARIO
#
rm -f ../embr/embr.pream.$SCENARIO
rm -f ../error/error.pream.$SCENARIO
rm -f ../msg/msg.pream.$SCENARIO
#
echo "---------------------------------------------------"
echo "    Running PREAM for $SCENARIO"
echo "---------------------------------------------------"
#
$EXEC/pream/pream << IEOF
USERIN file         :../inputs/userin.$SCENARIO
Input AMS file      :../inputs/AMS.area.$SCENARIO
Output Messages     :../msg/msg.pream.$SCENARIO
Output  EMBR        :../embr/embr.pream.$SCENARIO
EMAR error file     :../error/error.pream.$SCENARIO
IEOF
```

Exhibit 3-7. Example of a PREAM job script.

3.3 LBASE

The LBASE (**L**ink-**BASE**d emissions processor) module incorporates link-based emissions estimates into the modeling inventory; like the PREPNT and PREAM modules, LBASE serves as an entry point for the EPS3 system. The primary functions of the LBASE module are

    Identification of links within the modeling domain,

    Spatial allocation of link-based emissions to grid cells,

    Reformatting of link-based emissions estimates into the EMBR format.

LBASE reads link-specific emissions data, processes the data for each link, and writes the processed data to an EMBR file. The data may be hourly, seasonal, or annual average emission rates for criteria pollutants. If the input data contains annual or seasonal emissions, LBASE will divide the emissions by the number of days in the interval to calculate an average daily emissions rate. If the input data contains daily or hourly emissions, LBASE does not adjust the emissions rates.

Because the magnitude of emission rates found in a link-based emission inventory can vary greatly, the LBASE module allows for emissions rates to be in tons or grams. A flag in the

/LBASE/ packet of the USERIN file determines the units of the input link-based emissions file.

LBASE spatially allocates the link-based emissions by computing the fraction of the total link length contained in each cell traversed by the link.

> ➤ **Special Note**
> The user must ensure the location information in the link data is in the same coordinate system used for the modeling domain definition. The primary coordinate forms are geodesic, UTM and Lambert Conformal Projection (LCP). When using the LCP system, standard practice is to convert the LBASE coordinates outside of EPS3.

Data Validity Screening

Since LBASE is an entry point for the EPS3 system, the module performs various checks to identify missing or invalid data. First, LBASE compares the FIPS code on each input link emissions record with the county list found in the /COUNTY/ packet of the USERIN; any records with a county code not found in the list are not processed (i.e., not written to the EMBR file). Because the coordinate system used in the modeling application is arbitrary, it is not possible for the LBASE program to screen the link node coordinates for validity. It is up to the user to verify that the link nodes use the correct coordinate system and units.

Input Files

LBASE requires two input files: the USERIN file and the link-based emissions data file.

LBASE reads four packets from the USERIN file:

/LBASE/   This packet contains one item, a flag that indicates if the units of the input emissions are tons or grams. (Table 3-5) and (Exhibit 3-8).

/DATE/   LBASE reads the /DATE/ packet (Table 2-6) to obtain the date of the modeling episode. LBASE checks that the month and day of the modeling episode corresponds to the time period specified on each input AMS record.

/REGION/   LBASE reads this packet to obtain information regarding the definition of the modeling domain (Table 2-7). This information is required in order to correctly allocate the link-based emissions to grid cells.

/COUNTY/   This packet contains the list of counties within the modeling domain (Table 2-8). LBASE reads this packet to check the county identification code specified on each input record against the region county list.

/CRITERIA TABLES/ This packet specifies which output tables, if any, the user wants to include in the output message file (Table 2-11). See Section 2.4 for a full discussion on the output tables.

Table 3-5. /LBASE/ packet of EPS3 global user input file, USERIN.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	A	Packet identifier - /LBASE/
2		1-20		Not used
	CVTUNT	21-30	A	Flag which determines if input emissions are in TONS or GRAMS
3	KEYEND	1-20	A	Packet terminator - /END/

```
/LBASE/
Units of Input Emis:Grams
/END/
```

Exhibit 3-8. LBASE packet of USERIN.

The second input file required by LBASE is the link-based emissions file; Exhibit 3-9 shows a portion of a sample link-based emissions file. The first record of this file, which must begin with the keyword **Species**, indicates the order of the pollutants contained in the file. This mechanism allows LBASE to support a variable list of pollutants. The names of the pollutants used here must be listed in the /CRTERIA POLLUTANT/ packet of the USERIN file. Each data record of the link-based emissions file contains a single link segment, identified by the coordinates of the beginning and ending nodes of the link and the state/county FIPS code of the county containing the link (Table 3-6). Each record also contains information regarding vehicle class and road type (the classifications are the same as those employed in the AMS), emissions components (exhaust, evaporative, resting loss, or running loss), and criteria pollutant emissions for that link. The vehicle class and road type classifications are for reference only and are not used by the LBASE module. Each link must be contained entirely within a single county; in other words, links that cross county borders must be subdivided into sections until each section traverses only one county.

Table 3-6. Link-based motor vehicle emissions data file input into the LBASE module.

Line	Variable	Columns	Type	Description
1	CRTNAM	9-?	C	This line must begin with the keyword "Species", and is followed by the names (separated by spaces) of the pollutants contained in the file.
2+	FIPLNK	1-5	C	State/county code
	SICLNK	7-10	C	Standard Industrial Category (SIC)
	ASCLNK	12-21	C	Area Source Category (ASC)
	INVBEG	23-30	I	Beginning date/time of inventory (YYMMDDHH)
	INVEND	32-39	I	Ending date/time of inventory (YYMMDDHH)
	XCDBEG	41-50	R	X direction coordinate of beginning of link (m)
	YCDBEG	51-60	R	Y direction coordinate of beginning of link (m)
	XCDEND	61-70	R	X direction coordinate of end of link (m)
	YCDEND	71-80	R	direction coordinate of end of link (m)
	IZNLNK	82-83	I	UTM zone (or zero)
	IVCLAS	85-86	I	Vehicle class (not used)
	IRDTYP	88-89	I	Road type (not used)
	IEMTYP	91-92	I	Emissions type (not used)
	MSLNK(1)	94-103	R	Link emissions for species 1
	MSLNK(2)	104-113	R	Link emissions for species 2, etc.

Output Files

LBASE produces two output files. The first of these is a message file consisting of tables of emissions totals; Exhibit 3-10 contains an example LBASE message file. The first section of this file lists the input and output file names; this section is followed by a summary of the region definition information. The next section contains any warning or error messages generated during execution. The final section provides summary tables of emissions totals, the order of the reported pollutants is the same as specified in the input link data.

The second file created by LBASE is a gridded EMBR emissions file. This file is labeled "MOBILE" in the file header. This EMBR file is processed through the EPS3 system to perform the other tasks required of emissions processing, such as the application of control factors and chemical speciation. However, as is often the case with link-based emissions, the initial inventory may already contain hourly rates. In this case the temporal allocation step is unnecessary and the TMPRL module need not be run for the link-based inventory. However, even though the link-based EMBR file created by LBASE contains a gridded inventory, the GRDEM module still serves as the exit point for the inventory stream. In this case, the GRDEM program just acts as a reformatting tool.

Exhibit 3-11 shows a sample of an LBASE job script.

```
Species NOX VOC CO
48209 2201 MV01110EXH 99081300 99081301   206582.50-1085164.0 206582.50-1085164.0  0  1  0  0      0.133      0.069      0.822
48209 2201 MV01110EXH 99081300 99081301   206582.50-1085164.0 207345.30-1083625.0  0  1  0  0      5.720      2.996     35.464
48209 2201 MV01110EXH 99081300 99081301   206582.50-1085164.0 205905.20-1083590.0  0  1  0  0      6.026      3.156     37.361
48209 2201 MV01110EXH 99081300 99081301   200439.60-1103184.0 200855.10-1102603.0  0  1  1  0    122.945     45.524    569.450
48209 2201 MV01110EXH 99081300 99081301   200439.60-1103184.0 200127.00-1103476.0  0  1  1  0     75.435     27.932    349.393
48209 2201 MV01110EXH 99081300 99081301   200855.10-1102603.0 201132.70-1102212.0  0  1  1  0    122.418     45.271    563.151
48209 2201 MV01110EXH 99081300 99081301   200892.80-1102494.0 200411.30-1103143.0  0  1  1  0    149.784     55.453    693.209
48209 2201 MV01110EXH 99081300 99081301   200411.30-1103143.0 200296.20-1103274.0  0  1  1  0     34.313     12.993    177.980
48209 2201 MV01110EXH 99081300 99081301   193541.90-1110378.0 192967.30-1111000.0  0  1  1  0    206.489     84.496   1489.507
48209 2201 MV01110EXH 99081300 99081301   192967.30-1111000.0 191616.90-1112545.0  0  1  1  0    502.755    205.730   3626.620
48209 2201 MV01110EXH 99081300 99081301   193656.80-1110285.0 193001.80-1110992.0  0  1  1  0    233.408     95.512   1683.683
48209 2201 MV01110EXH 99081300 99081301   193001.80-1110992.0 192694.70-1111354.0  0  1  1  0    117.718     48.171    849.157
48209 2201 MV01110EXH 99081300 99081301   195109.20-1108695.0 194675.60-1109172.0  0  1  1  0    151.866     58.270    838.556
48209 2201 MV01110EXH 99081300 99081301   195566.30-1108159.0 195052.40-1108723.0  0  1  1  0    153.687     56.830   1971.23
48209 2201 MV01110EXH 99081300 99081301   196100.10-1107604.0 195700.90-1108038.0  0  1  1  0    153.171     62.678   1104.899
48209 2201 MV01110EXH 99081300 99081301   197728.50-1105849.0 198396.00-1105119.0  0  1  1  0    244.755     93.900   1350.686
48209 2201 MV01110EXH 99081300 99081301   198396.00-1105119.0 198728.60-1104769.0  0  1  1  0     92.362     36.175    558.820
48209 2201 MV01110EXH 99081300 99081301   198512.20-1104970.0 197944.10-1105584.0  0  1  1  0    140.445     53.919    777.507
48209 2201 MV01110EXH 99081300 99081301   197944.10-1105584.0 197482.60-1106082.0  0  1  1  0    152.352     58.234    625.994
```

Exhibit 3-9. Example of link-based emissions file used as input to LBASE.

```
            EPS3 LBASE module v. 1.00 Aug 2004        07/25/07 18:41:32

            Input Files
    USERIN file                        :../inputs/userin.test_problem.Hays
    link emissions file                :../inputs/LBASE_inputs.test_problem.Hays.990813

        Output Files
    Output EMBR file                   :../embr/embr.lbase.test_problem.Hays.990813


                EPS3 LBASE module v. 1.00 Aug 2004        07/25/07 18:41:32

    File note                          :CAMx Modeling of Tx regional, 9/13/99
    Episode date (Calander)            :990913
    Episode date (Julian)              :99256
    Beginning time                     :     0
    Ending time                        :    24
    Grid origin (km)                   : (  -108.000, -1584.000)
    UTM zone                           :     0
    Grid cell width (km)               : (    12.000,    12.000)
    Number of cells                    : (  135,  138)
    Number of counties                 :     1

                Total Emissions Processed
                    English Tons/Day


                        NOX         VOC         CO
        ----------------------------------------------------------
        Input Emissions        3.0787      1.2982      18.8145
        Output Emissions       3.0787      1.2982      18.8145
        Emissions Skipped      0.          0.          0.
        ----------------------------------------------------------



                    Criteria Emissions by Source Category and Hour
                                English Tons/Day


    Source Category   Hour     Input       Output      Input       Output      Input
        Output
                               NOX         NOX         VOC         VOC         CO
            CO
    ------------------------------------------------------------------------------------
        2201001110      01      0.0288      0.0288      0.0119      0.0119      0.1794
        2201001110      02      0.0179      0.0179      0.0074      0.0074      0.1111
        2201001110      03      0.0154      0.0154      0.0062      0.0062      0.0941
        2201001110      04      0.0120      0.0120      0.0049      0.0049      0.0746
```

Exhibit 3-10. Example of a LBASE message file.

```
#!/bin/csh
#
#    --- Sample job script for running the
#        EPS3 module LBASE
#
set EXEC = /models/eps3.devel/src
#
set SCENARIO = test_problem.Hays
set DAY = 990813
#
rm -f ../msg/msg.lbase.$SCENARIO.$DAY
rm -f ../embr/embr.lbase.$SCENARIO.$DAY
#
#
echo "---------------------------------------------------"
echo "    Running LBASE for $SCENARIO $DAY"
echo "---------------------------------------------------"
#
$EXEC/lbase/lbase << IEOF
USERIN file        :../inputs/userin.$SCENARIO
Input AMS file     :../inputs/LBASE_inputs.$SCENARIO.$DAY
Output Messages    :../msg/msg.lbase.$SCENARIO.$DAY
Output Mobile EMBR :../embr/embr.lbase.$SCENARIO.$DAY
IEOF
```

Exhibit 3-11. Example of a LBASE job script.

3.4 PREFIR

The PREFIR (**PRE**processor for point **FIR**e source emissions) module is the entry point to EPS3 for point specific fire source emissions data. The primary functions of PREFIR are

Identification of sources within the modeling domain,

Determine the fire class size of each source,

Optionally combine multiple sources in a grid cell, and

Reformat the input fire source emissions inventory into EMBR format.

PREFIR provides a mechanism to process fire emissions that have been reported at a fine resolution. Gridded satellite data can be processed prior to PREFIR in order to generate location specific fire source emission estimates.   These data are typically recorded as day-specific observed data. As such, through PREFIR, they are reformatted to EMBR format for speciation and temporal allocation. Each fire source emissions EMBR record is designated a fire source with the letter "F" as the record type.   Following speciation and temporal allocation the source specific fire source emissions will be processed by PSTFIR which generates the inventory output files; both the CAMx surface file and elevated point source files for merging in PIGEMS.

PREFIR reads fire source input emissions which include state/county code, SCC code, fire code, fire group code, time period, fire virtual acreage, pollutant code and emissions estimate. The fire and group codes may be thought of as plant and stack identifiers and may be used for reporting.

The virtual acreage indicates the fire size which determines the parameters that are used for computing the fraction of emissions at the surface and the top and bottom of the plume in the PSTFIR module. The input emissions file may include any criteria pollutant codes specified in the /CRITERIA POLLUTANT/ packet of the USERIN.

As already stated, typically the point specific emissions are represented as a specified date. However, PREFIR does support the additional emission periods that the other EPS3 entry modules support. For a complete discussion of annual, seasonal, peak ozone, peak CO, or other specified periods refer to Section 3.1 PREPNT.

> ➢ **Special Note**
> PREFIR will consolidate multiple emission records which are from a single source if the data are arranged consecutively in the input file. Prior to running PREFIR, the data should be sorted using the following UNIX sort command:
> :
> sort -o <*SORTED_OUTPUT_FILE*> <*INPUT_FILE*>
>
> This assumes that all criteria pollutants from a single fire source share the same fire and group identifiers. This step will result in a smaller EMBR output file and efficient execution of subsequent EPS3 modules and utilities.

Fire Source Screening

PREFIR, as an EPS3 input module, screens the input data to determine which point-specific fire source emissions records fall within the modeling domain. This determination is based on the region definition provided in the /REGION/ packet of the USERIN. In addition, the state/county identification codes are checked against the user-supplied county list (specified in the /COUNTY/packet of the USERIN) to ensure that the correct region is included in the input fire source inventory file. A message is written to the message output file indicating which counties in the county list had no corresponding data records.

The virtual acreage of the fire source dictates the fire size class. If the virtual acreage is missing from the input record one of two things may happen; either a default fire class is assigned or the record is written to the error output file. The outcome depends on user parameters specified in the /PREFIR/ packet of the USERIN. If the option to process missing acreage data is set to "YES", PREFIR sets the fire class size to the user specified default fire class size and continues processing. If this option is set to "NO", the record is not processed (i.e., not written to EMBR), but rather is written to a separate error file (this file may be empty if all of the fire source data is determined to be acceptable). The PREFIR module sets the EMBR record stack diameter field to the fire class size which is used in PSTFIR for vertical distribution of emissions.

The default fire class size parameters are indicated in Table 3-7. These parameters are taken from the WRAP 2002 Phase II EI Report (22 July 2005). A user may override these defaults with the /FIRE BINS/ packet in the USERIN file discussed in detail below. Any changes to these classifications should be made under the guidance of expert opinion.

Table 3-7. Default fire class parameters for both /PREFIR/ and PSTFIR modules.

Fire Class	Size (virtual acres)	Buoyant Efficiency	Plume top max (m)	Plume bottom max (m)
1	0 -10	0.40	160	0
2	>=10 – 100	0.60	2,400	900
3	>= 100 – 1,000	0.75	6,400	2,200
4	>= 1,000 – 5,000	0.85	7,200	3,000
5	>= 5,000	0.90	8,000	3,000

Combining Fire Sources

Due to the fine resolution of satellite fire data the input fire source emissions may be at a much finer resolution than required for the modeling application. In order to reduce the number of processing records, thereby optimizing processing time and space, PREFIR has an option to combine sources within a grid cell. Typically a grid cell refers to the modeling region definition cell size specified in the USERIN /REGION/ packet. However, for purposes of combining fire sources over a very large modeling domain, for example the RPO national domain at 36km resolution, the user may choose to combine points at a smaller resolution, perhaps 12km or 4km. This would reduce the number of fire source records to process at the same time as maintaining a finer resolution for nested grids. This can be accomplished through the /PREFIR/ packet of the USERIN.

If a user specifies "YES" to the combine fire sources flag and provides a grid resolution then PREFIR will combine sources prior to writing the output EMBR file. Fire sources will be combined only if they fall within a single 'fine' resolution grid cell, have the same state/county code, have the same SCC code, and have the same fire class size. If sources are combined PREFIR will assign a new fire identifier of "Fnnn" where nnn is a unique sequential number and the group code will be assigned "Smmm" where mmm represents the count of input sources that have been combined.

Input Files

PREFIR requires two input files: the user input file USERIN and the input fire source inventory. PREFIR reads the following packets from USERIN.

/PREFIR/   The /PREFIR/ packet contains the input parameters unique to the PREFIR program. (Table 3-8). This includes the user options for input coordinates in either geodesic or UTM coordinates, a flag that indicates if missing fire acreage data should be processed, the default fire class size to assign missing acreage data, a flag to indicate if fire sources should be combined by grid cell, and the cell resolution for combining sources. (Exhibit 3-12)

Table 3-8. /PREFIR/ packet of EPS3 global user input file, USERIN.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	C	Packet identifier - /PREFIR/
2		1-20		Not used
	LGEODS	21-30	C	Flag which determines if input coordinates are to be converted: YES = input coordinates are geodesic and should be converted NO = input coordinates match modeling domain and should not be converted
3		1-20		Not used
	LPRCES	21-30	C	Flag which determines if missing fire size data are processed: YES = process data with missing fire acreage NO = write record to error file and skip
4		1-20		Not used
	IBINDF	21-30	I	Default fire class size for fire sources with missing acreage.
5		1-20		Not used
	LCOMB	21-30	C	Flag which determines if fire source emissions should be combined within grid cells. YES = combine source emissions NO = do not combine fire sources
6		1-20		Not used
	DXCOMB	21-30	R	Cell resolution for combining sources (meters)
7	KEYEND	1-20	A	Packet terminator - /END/

```
/PREFIR/
GEODESIC COORDINATE: NO
PROCES MSNG ACREAGE: YES
DEFAULT BIN        : 2
COMBINE POINTS     : yes
Combine dxy  (km) : 4.
/END/
```

Exhibit 3-12. /PREFIR/ packet of USERIN.

/FIRE BINS/ PREFIR reads the /FIRE BINS/ packet (Table 3-9). If the packet is not provided then the defaults specified in Table 3-7 will be used. This packet allows the user to specify different fire class definitions. The fire sizes must be provided in increasing value. When determining a source fire size PREFIR searches the list from beginning to end. As soon as it finds a fire size bin less than the virtual acreage of the fire it sets the fire class to that level. Exhibit 3-13 is an example of the /FIRE BINS/ packet specifying the default parameters.

Table 3-9. /FIRE BINS/ packet of EPS3 global user input file, USERIN.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	C	Packet identifier - /FIRE BINS/
2+		1-20		Not used
	SIZFBIN	21 - *	R	Maximum acreage (virtual acres)
	BEFBIN		R	Buoyant efficiency
	TOPFBIN		R	Plume top maximum (m)
	BOTFBIN		R	Plume bottom maximum (m)
3	KEYEND	1-20	A	Packet terminator - /END/

* The fire bin records are free format, space delimited fields.

```
/FIRE BINS/
Fire class 1        :       10    0.40    160.      0.
Fire class 2        :      100    0.60   2400.    900.
Fire class 3        :     1000    0.75   6400.   2200.
Fire class 4        :     5000    0.90   8000.   3000.
/END/
```

Exhibit 3-13. /FIRE BINS/ packet of USERIN.

/CRITERIA POLLUTANT/ PREFIR reads this packet (Table 2-9) to determine which of the input pollutants to include in the modeling inventory. The criteria pollutants will be stored on the EMBR record in the same order they appear in the packet.

/DATE/   PREFIR reads the /DATE/ packet (Table 2-6) to obtain the date of the modeling episode. For period-specific input files, PREFIR checks that the month and day of the modeling episode corresponds to the time period specified on each input record.

/REGION/   This packet contains the definition of the modeling domain (Table 2-7) and allows PREFIR to exclude those fire sources located outside of the modeling region, thus reducing the computer processing time required by subsequent modules.

/COUNTY/ This packet contains the list of counties within the modeling domain (Table 2-8). PREFIR reads this packet to check the county identification code specified on each input record against the modeling region county list, and to determine if any specified counties had no corresponding data records, i.e., identify possible missing input emission data. The /COUNTY/ packet also contains county time zone designation.

/CRITERIA TABLES/ This packet specifies which output tables, if any, the user wants to include in the output message file (Table 2-11). See Section 2.4 for a full discussion on the output tables. Since the emissions input to PREFIR are not typically speciated, the /SPECIES TABLES/ packet is not read.

The second input file is the fire source emissions file. The format of this file is specified in Table 3-10 with an example provided in Exhibit 3-14.

Table 3-10. Fire source emissions input into the PREFIR module.

Line	Variable	Columns	Type	Description
1+	INFIPS	12-16	C	State/county code
	INSCC	29-38	C	Source Classification Code (SCC)
	INPLNT	40-49	C	Fire identification code
	INSTCK	51-60	C	Fire-group identification code
	IPEROD	77-78	C	Period Type Blank = Annual 　PO = Peak O_3 typical weekday 　PC = Peak CO typical weekday 　AD = Average Day 　S　= Specified interval
	IBEGDT	80-87	I	Beginning period interval date/time; time is in military format (YYMMDDHH)
	IENDDT	89-96	I	Ending period interval date/time; time is in military format (YYMMDDHH). Note: the time interval stops at the <u>start</u> of the specified end hour.
	XLOC	98-107	R	Latitude (decimal degrees) or Easting coordinate (km) to define location of fire source
	YLOC	109-118	R	Longitude (decimal degrees) or Northing coordinate (km) to define location of fire source
	IZONE	120-121	I	UTM zone associated with UTM coordinates (optional if location is lat/lon)
	ACREAGE	123-127	R	Virtual area of fire (acres)
	INPOL	176-180	I	Pollutant code
	CRTPOL	182-191	R	Emissions of specified pollutant Units depend on the Period Type Annual = tons/year PO/PC = tons/typical weekday AD = tons/average day S = tons/period (the period is specified using the beginning and ending time fields)

> ➢ **Special Note**
> PREFIR, like PREPNT, manipulates the input geographical coordinates based on the coordinate flag in the /PREFIR/ packet. The user must ensure the location information is in the same coordinate system used for the modeling application. The primary coordinate forms are geodesic, UTM and Lambert Conformal Projection (LCP). When using the LCP system, standard practice is to convert the fire source coordinates outside of EPS3 and set the "convert Coordinates" flag to "No".

```
48000 2810001000 F15460    I15460    S  05060500 05060524     204.270   -1139.900       47.1 42101    34.6354    CO     Texas
48000 2810001000 F15460    I15460    S  05060500 05060524     204.270   -1139.900       47.1 81102     3.4288    PM10   Texas
48000 2810001000 F15460    I15460    S  05060500 05060524     204.270   -1139.900       47.1 81104     2.8325    PM25   Texas
48000 2810001000 F15460    I15460    S  05060500 05060524     204.270   -1139.900       47.1 42603     1.1926    NOx    Texas
48000 2810001000 F15460    I15460    S  05060500 05060524     204.270   -1139.900       47.1 42604     0.7454    NH3    Texas
48000 2810001000 F15460    I15460    S  05060500 05060524     204.270   -1139.900       47.1 42401     0.1988    SO2    Texas
48000 2810001000 F15460    I15460    S  05060500 05060524     204.270   -1139.900       47.1 43104     3.3294    VOC    Texas
48000 2810001000 F15460    I15460    S  05060500 05060524     204.270   -1139.900       47.1 12142     0.0001    Hg     Texas
CA10  2810001000 F15461    G00001    S  05060500 05060524    2250.650   1741.627       3550.3 42101   494.5941    CO     Quebec
CA10  2810001000 F15461    G00001    S  05060500 05060524    2250.650   1741.627       3550.3 81102    73.2111    PM10   Quebec
CA10  2810001000 F15461    G00001    S  05060500 05060524    2250.650   1741.627       3550.3 81104    67.6225    PM25   Quebec
CA10  2810001000 F15461    G00001    S  05060500 05060524    2250.650   1741.627       3550.3 42603    13.9716    NOx    Quebec
CA10  2810001000 F15461    G00001    S  05060500 05060524    2250.650   1741.627       3550.3 42604     5.0298    NH3    Quebec
CA10  2810001000 F15461    G00001    S  05060500 05060524    2250.650   1741.627       3550.3 42401     4.4709    SO2    Quebec
CA10  2810001000 F15461    G00001    S  05060500 05060524    2250.650   1741.627       3550.3 43104    34.0907    VOC    Quebec
CA10  2810001000 F15461    G00001    S  05060500 05060524    2250.650   1741.627       3550.3 12142     0.0018    Hg     Quebec
CA10  2810001000 F15462    G00002    S  05060500 05060524    1368.981   1472.537       1567.4 42101   101.0004    CO     Quebec
CA10  2810001000 F15462    G00002    S  05060500 05060524    1368.981   1472.537       1567.4 81102    14.0278    PM10   Quebec
CA10  2810001000 F15462    G00002    S  05060500 05060524    1368.981   1472.537       1567.4 81104    10.6612    PM25   Quebec
```

Exhibit 3-14. Example of a PREFIR input emissions.

Output Files

The PREFIR program produces the output files: the PREFIR message file, an EMBR file, and an error file containing input records that PREFIR was unable to process due to errors.

The first section of the PREFIR message file, Exhibit 3-15, summarizes input and output file names, episode and region definition parameters, and the fire class bin parameters. This section is followed by a summary of the number of records processed, the domain-wide criteria pollutant emissions totals for the input and output files, and warning messages indicating counties in the /COUNTY/ packet of USERIN for which no records were found in the input fire source file. The final section of the PREFIR message file consists of summary tables selected by the user in the /CRITERIA TABLES/ packet of USERIN.

The second output file is the point source emissions inventory EMBR file, with a specified file type of "FIRPTS" in the header records.

The third output file, which may be empty, contains the input fire data records which have insufficient data for processing. This file is written in the same format as the input file format to facilitate review, correction, and reprocessing.

Exhibit 3-16 shows a sample of a PREFIR job script.

```
                    EPS3 PREFIR module v. 1.00 Jun 2008


              Input Files
           USERIN file                  :../../inputs/userin.regional_fires
           Input data file              :../../inputs/fire_pts.2005_0605.srt


              Output Files
           Output msg file              :msg.prefir.2005_0605
           Output EMBR file             :embr.prefir.2005_0605
           ERROR file                   :emar.prefir.2005_0605


                    EPS3 PREFIR module v. 1.00 Jun 2008      08/20/08 10:21:49


           File note                    :CAMx Fires Test Case
           Episode date (Calander)      : 50605
           Episode date (Julian)        : 5156
           Beginning hour               :    0
           Ending hour                  :   24
           Grid origin (km)             : (  -108.000, -1584.000)
           UTM zone                     :    0
           Grid cell width (km)         : (    36.000,    36.000)
           Number of cells              : (  69,   67)
           Number of counties           :   96
           Specified Fire Bins          : None - Defaults Assigned
                                          Class    Size       BE  PtopMax  PbotMax
                                            1      10.0    0.400   160.0      0.0
                                            2     100.0    0.600  2400.0    900.0
                                            3    1000.0    0.750  6400.0   2200.0
                                            4    5000.0    0.850  7200.0   3000.0
                                            5    9999.0    0.900  8000.0   3000.0
           Geodesic coordinates         :NO
           Process missing fire acreage :YES
           Default fire class           :    2
           Combine point sources        :YES
           Combining resolution (km)    :  4.000

Number of input records read:    1206
Number of input records written to EMAR:        0
Number of input records skipped:    934
Number of input to output records:     272
Number of output EMBR records:      27
                                        Total Emissions Processed
                                            English Tons/Day


                     NOX         VOC         CO          SO2          NH3          SO4
          -------------------------------------------------------------------------------------
Input Emissions      0.137E+05   0.298E+05   0.451E+06   3799.2196   4255.0629      0.
 Output Emissions     127.4548    280.4266   3934.4087     32.1956     40.1360       0.
 Outside Region       0.136E+05   0.295E+05   0.447E+06   3767.0240   4214.9269      0.
 Written to ERR file     0.          0.          0.          0.          0.          0.
 Total Skipped        0.136E+05   0.295E+05   0.447E+06   3767.0240   4214.9269      0.
          -------------------------------------------------------------------------------------


     County 09000 contained no emissions in input file.
     County 10000 contained no emissions in input file.    …
```

Exhibit 3-15. Example of a PREFIR message file.

```
#!/bin/csh
#
#   --- Sample job script for running the
#       EPS3 module PREFIR
#
set EXEC = /models/eps3/src
#
set SCENARIO = test_problem
#
# --- sort the input fire source emissions file ---
#
sort -o ../inputs/fire_pts.$SCENARIO.srt ../inputs/fire_pts.$SCENARIO
#
#
rm -f ../msg/msg.prefir.$SCENARIO
rm -f ../embr/embr.prefir.$SCENARIO
rm -f ../error/error.prefir.$SCENARIO
#
echo "-------------------------------------------------"
echo "    Running PREFIR for $SCENARIO"
echo "-------------------------------------------------"
#
$EXEC/prefir/prefir << IEOF
USERIN file        :../inputs/userin.$SCENARIO
Input fire file    :../inputs/fire_pts.$SCENARIO.srt
Output Messages    :../msg/msg.prefir.$SCENARIO
Output EMBR        :../embr/embr.prefir.$SCENARIO
EMAR error file    :../error/error.prefir.$SCENARIO
IEOF
```

Exhibit 3-16. Example of a PREFIR job script.

3.5 PRESHP

The PRESHP (**PRE**processor for **SHiP**ping emissions) module incorporates shipping emissions estimates within shipping lanes into the modeling inventory; like the PREPNT and PREAM modules, PRESHP serves as an entry point for the EPS3 system. The primary functions of the PRESHP module are

Identification of shipping channels within the modeling domain,

Spatial allocation of shipping channel emissions to grid cells,

Reformatting of shipping emissions estimates into the EMBR format.

PRESHP reads shipping lane emissions data, processes the data for each lane, and writes the processed data to an EMBR file. The data may be hourly, seasonal, or annual average emission rates for criteria pollutants. If the input data contains annual or seasonal emissions, PRESHP will divide the emissions by the number of days in the interval to calculate an average daily emissions rate. If the input data contains daily or hourly emissions, PRESHP does not adjust the emissions rates.

The shipping lane is defined by the end point coordinates of the lane center line and the lane width at the beginning and end points. The lane center in Figure 3-1 below is depicted by the line AB. The lane width is specified by the distance C at endpoint A, and distance D at endpoint B. PRESHP spatially allocates the shipping lane emissions by first allocating the emissions to the cells along the shipping lane center line AB, similar to LBASE. Then each center line cell estimate is further distributed to the cells in the perpendicular direction from the center line to the lane boundaries. This ensures that higher density emissions occur in cells at the narrower lane mouths typically near ports.

Table 3-? Variables:
A – coordinates of shipping lane beginning XLOCBEG, YLOCBEG
B – coordinates of shipping lane end XLOCEND, YLOCEND
C - lane width at endpoint A, WIDEBEG
D - lane width at endpoint B, WIDEEND
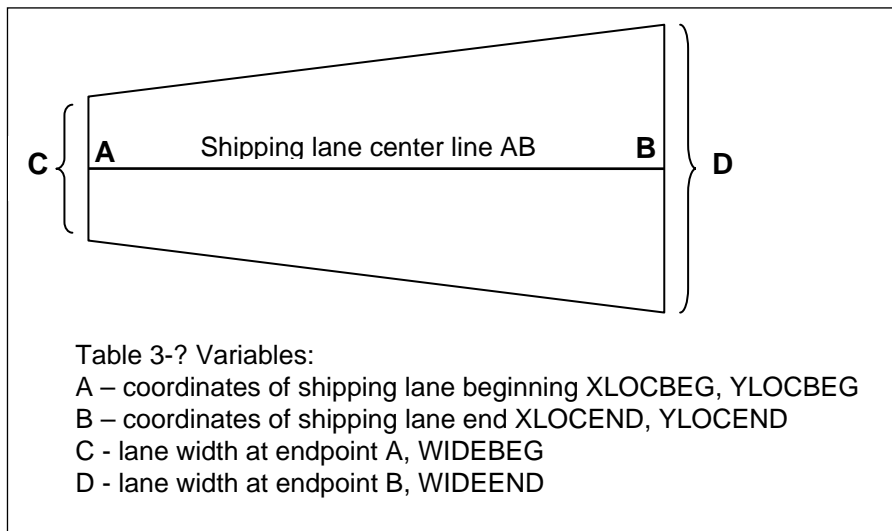
Figure 3-1. PRESHP shipping lane parameters.

Some existing shipping lane inventories are pre-gridded in a GIS system and reported as 'point' sources. These data can be processed in PRESHP by defining the the point A equal to the point B which will result in a zero length shipping lane. These point source shipping emissions will be gridded to a single grid cell.

Data Validity Screening

Since PRESHP is an entry point for the EPS3 system, the module performs various checks to identify missing or invalid data. First, PRESHP checks for a valid pollutant code. Next it compares the FIPS code on each input emissions record with the county list found in the /COUNTY/ packet of the USERIN; any records with a county code not found in the list are not processed (i.e., not written to the EMBR file). Shipping lanes often fall outside of standard county borders. In this case, the FIPS code may be any five (or less) character code used to identify the shipping lane. During spatial allocation any portion of a shipping lane that falls outside of the modeling domain are dropped. Because the coordinate system used in the modeling application is arbitrary, it is not possible for the PRESHP program to screen the lane node coordinates for validity. It is up to the user to verify that the lane nodes use the correct coordinate system and units. The coordinate system must be rectangular, typically LCP or UTM, the geodesic system is not supported.

Input Files

PRESHP requires two input files: the USERIN file and the shipping lane emissions data file.

PRESHP reads five packets from the USERIN file:

/CRITERIA POLLUTANT/ PREAM reads this packet (Table 2-9) to determine which of the input pollutants to include in the modeling inventory. The criteria pollutants will be stored on the EMBR record in the same order they appear in the packet.

/DATE/   PRESHP reads the /DATE/ packet (Table 2-6) to obtain the date of the modeling episode. PRESHP checks that the month and day of the modeling episode corresponds to the time period specified on each input record.

/REGION/   PRESHP reads this packet to obtain information regarding the definition of the modeling domain (Table 2-7). This information is required in order to correctly allocate the shipping lane emissions to grid cells.

/COUNTY/ This packet contains the list of counties within the modeling domain (Table 2-8). PRESHP reads this packet to check the county identification code specified on each input record against the region county list.

/CRITERIA TABLES/ This packet specifies which output tables, if any, the user wants to include in the output message file (Table 2-11). See Section 2.4 for a full discussion on the output tables.

The second input file is the shipping emission estimates specified by shipping lane (Table 3-11). A sample shipping input file is shown in Exhibit 3-17.

Table 3-11. Shipping emissions data input into the PRESHP module.

Line	Variable	Columns	Type	Description
1+	INFIPS	1-5	C	State/county/shipping lane code
	INSBRG	7-11	C	Subregion code (optional)
	INSCC	13-22	C	Source Classification Code (SCC)
	INVESL	24-33	C	Vessel type code (optional)
	IPEROD	35-36	C	Period Type Blank = Annual PO = Peak O_3 typical weekday PC = Peak CO typical weekday AD = Average Day S = Specified interval
	IBEGDT	38-45	I	Beginning period interval date/time; time is in military format (YYMMDDHH)
	IENDDT	47-54	I	Ending period interval date/time; time is in military format (YYMMDDHH). Note: the time interval stops at the <u>start</u> of the specified end hour.
	XLOCBEG	56-65	R	X coordinate of beginning of channel link (km)
	YLOCBEG	67-76	R	Y coordinate of beginning of channel link (km)
	WIDEBEG	78-87	R	Channel width at beginning of channel (km)
	XLOCEND	89-98	R	X coordinate of end of channel link (km)
	YLOCEND	100-109	R	Y coordinate of end of channel link (km)
	WIDEEND	111-120	R	Channel width at end of channel (km)
	INZONE	122-123	I	UTM Zone (or zero)
	INPOL	125-129	I	Pollutant Code
	EMSSHIP	131-140	R	Emissions of specified pollutant Units depend on the Period Type Annual = tons/year PO/PC = tons/typical weekday AD = tons/average day S = tons/period (the period is specified using the beginning and ending time fields)

> **Special Note**
The user must ensure the location information of the lane definition is in the same coordinate system used for the modeling domain definition. The primary coordinate forms are UTM and Lambert Conformal Projection (LCP).

```
BD01  101 2280003d11 Bulk Cargo   02010100 02123123  481.4692 -1120.9789  0.16  482.4692 -1120.9789  0.189 0 42603  0.00073
BD01  102 2280003d11 Bulk Cargo   02010100 02123123  482.4270 -1120.7306  0.16  483.4270 -1120.7306  0.189 0 42603  0.00073
BD01  101 2280003d11 Bulk Cargo   02010100 02123123  481.4692 -1120.9789  0.16  482.4692 -1120.9789  0.189 0 43104  0.00002
BD01  102 2280003d11 Bulk Cargo   02010100 02123123  482.4270 -1120.7306  0.16  483.4270 -1120.7306  0.189 0 43104  0.00002
BD01  101 2280003d13 Container    02010100 02123123  481.4692 -1120.9789  0.16  482.4692 -1120.9789  0.189 0 42101  0.00793
BD01  102 2280003d13 Container    02010100 02123123  482.4270 -1120.7306  0.16  483.4270 -1120.7306  0.189 0 42101  0.00793
BD01  101 2280003d13 Container    02010100 02123123  481.4692 -1120.9789  0.16  482.4692 -1120.9789  0.189 0 42603  0.05197
BD01  102 2280003d13 Container    02010100 02123123  482.4270 -1120.7306  0.16  483.4270 -1120.7306  0.189 0 42603  0.05197
BD01  101 2280003d13 Container    02010100 02123123  481.4692 -1120.9789  0.16  482.4692 -1120.9789  0.189 0 43104  0.00131
BD01  102 2280003d13 Container    02010100 02123123  482.4270 -1120.7306  0.16  483.4270 -1120.7306  0.189 0 43104  0.00131
BD01  101 2280003d14 Liquefied    02010100 02123123  481.4692 -1120.9789  0.16  482.4692 -1120.9789  0.189 0 42101  0.01106
BD01  102 2280003d14 Liquefied    02010100 02123123  482.4270 -1120.7306  0.16  483.4270 -1120.7306  0.189 0 42101  0.01106
BD01  101 2280003d14 Liquefied    02010100 02123123  481.4692 -1120.9789  0.16  482.4692 -1120.9789  0.189 0 42603  0.06099
BD01  102 2280003d14 Liquefied    02010100 02123123  482.4270 -1120.7306  0.16  483.4270 -1120.7306  0.189 0 42603  0.06099
BD01  101 2280003d14 Liquefied    02010100 02123123  481.4692 -1120.9789  0.16  482.4692 -1120.9789  0.189 0 43104  0.00141
BD01  102 2280003d14 Liquefied    02010100 02123123  482.4270 -1120.7306  0.16  483.4270 -1120.7306  0.189 0 43104  0.00141
BD01  101 2280003d15 Oil/Chemic   02010100 02123123  481.4692 -1120.9789  0.16  482.4692 -1120.9789  0.189 0 42101  0.05655
BD01  102 2280003d15 Oil/Chemic   02010100 02123123  482.4270 -1120.7306  0.16  483.4270 -1120.7306  0.189 0 42101  0.05655
BD01  101 2280003d15 Oil/Chemic   02010100 02123123  481.4692 -1120.9789  0.16  482.4692 -1120.9789  0.189 0 42603  0.29121
BD01  102 2280003d15 Oil/Chemic   02010100 02123123  482.4270 -1120.7306  0.16  483.4270 -1120.7306  0.189 0 42603  0.29121
BD01  101 2280003d15 Oil/Chemic   02010100 02123123  481.4692 -1120.9789  0.16  482.4692 -1120.9789  0.189 0 43104  0.00776
BD01  102 2280003d15 Oil/Chemic   02010100 02123123  482.4270 -1120.7306  0.16  483.4270 -1120.7306  0.189 0 43104  0.00776
BD01  101 2280003d17 Cruise Shi   02010100 02123123  481.4692 -1120.9789  0.16  482.4692 -1120.9789  0.189 0 42101  0.07068
BD01  102 2280003d17 Cruise Shi   02010100 02123123  482.4270 -1120.7306  0.16  483.4270 -1120.7306  0.189 0 42101  0.07068
BD01  101 2280003d17 Cruise Shi   02010100 02123123  481.4692 -1120.9789  0.16  482.4692 -1120.9789  0.189 0 42603  0.36671
BD01  102 2280003d17 Cruise Shi   02010100 02123123  482.4270 -1120.7306  0.16  483.4270 -1120.7306  0.189 0 42603  0.36671
```

Exhibit 3-17. Example of shipping lane emissions input file to PRESHP.

Output Files

The PRSHP program produces three output files: a message file, an EMBR file, and an error file.

The first section of the message output file summarizes the input and output file names and provides information regarding the input shipping emissions file and user-defined modeling region. The next section summarizes domain-wide input and output emissions totals and totaled processed emission outputs for criteria pollutants and lists any counties specified in the /COUNTY/ packet of the USERIN file for which no emissions records were found. The final section of the message output file includes summary tables selected in the USERIN /CRITERIA TABLES/ packet. Exhibit 3-18 shows a sample of a PRESHP message file.

PRSHP creates an EMBR file containing emissions records for the sources included in the input emissions file that pass all data validity checks.

The third output file will contain data only if PRESHP encounters records with insufficient data for processing. PRESHP writes these records to a separate file in the same format as input in order to facilitate reprocessing of the data once corrections have been made.

Exhibit 3-19 shows a sample PRESHP job script.

```
                    EPS3 PRESHP module v. 3.12 Apr 2009

            Input Files
        USERIN file                     :./userin.hg_bpa.shipping
        Input SHIPS file                :../data/hg+bpa_lcp_ships.fy2005a.preshp

            Output Files
        Output msg file                 :../msg/msg.preshp.2km.tx.hg+bpa_ships
        Output EMBR file                :../embr/embr.preshp.2km.tx.hg+bpa_ships
        ERROR file                      :../error/error.preshp.2km.tx.hg+bpa_ships


            EPS3 PRESHP module v. 3.11 Apr 2009     07/14/09 13:53:28


        File note                       :TX CAMx Modeling hous_2km
        Episode date (Calander)         : 20601
        Episode date (Julian)           : 2152
        Beginning hour                  :    0
        Ending hour                     :   24
        Grid origin (km)                : (    400.000,  -1200.000)
        UTM zone                        :    0
        Grid cell width (km)            : (     2.000,     2.000)
        Number of cells                 : ( 180,  100)
        Number of counties              :   29

Number of input records read:     10179

Number of input records written to error file:         9

Number of input records skipped:         9

Number of output records written:     9138

                    Total Emissions Processed
                       English Tons/Day

                       NOX          CO          VOC          SO2
    ----------------------------------------------------------------------
    Input Emissions       0.0911      0.0123      0.0028       0.
    Output Emissions      0.0910      0.0123      0.0028       0.
    Outside Region     0.618E-04   0.625E-05   0.181E-05       0.
    Written to ERR file    0.          0.          0.          0.
    Total Skipped      0.618E-04   0.625E-05   0.181E-05       0.
    ----------------------------------------------------------------------

        County RSZON contained no emissions in input file.
        County STEEM contained no emissions in input file.

                    Criteria Pollutant Emissions by County
                             English Tons/Day


    County     Input      Output      Input      Output      Input      Output
               NOX        NOX         CO         CO          VOC        VOC
    ----------------------------------------------------------------------------
      BD01     0.0042     0.0042      0.0008     0.0008      0.0001    0.793E-04
      BT01     0.0043     0.0043      0.0005     0.0005      0.0001     0.0002
      FD01     0.0026     0.0026      0.0005     0.0005     0.660E-04  0.341E-04
      FT01     0.0002     0.0002    0.250E-04  0.187E-04   0.718E-05  0.384E-04
      GD01     0.0018     0.0018      0.0003     0.0003    0.461E-04  0.378E-04
      GT01     0.0006     0.0006    0.565E-04  0.565E-04   0.162E-04  0.234E-04
      HD01     0.0018     0.0018      0.0003     0.0003    0.464E-04  0.447E-04
      HD02     0.0013     0.0013      0.0003     0.0003    0.359E-04  0.368E-04
      HD03     0.0094     0.0094      0.0017     0.0017      0.0002     0.0002
        .
        .
        .
    ----------------------------------------------------------------------------
    Total      0.0911     0.0910      0.0123     0.0123      0.0028     0.0028
```

Exhibit 3-18. Example of a PRESHP message file.

ENVIRON

```
#!/bin/csh
#
#   --- Sample job script for running the
#       EPS3 module PRESHP
#
set EXEC = /models/eps3/src
#
set SCENARIO = hgbpa_shipping.fy2005a
#
# --- sort the input shipping source emissions file ---
#
sort -o ../data/hg+bpa_lcp_ships.fy2005a.preshp ./data/hg+bpa_ships.fy2005.dat
#
#
rm -f ../msg/msg.preshp.$SCENARIO
rm -f ../embr/embr.preshp.$SCENARIO
rm -f ../error/error.preshp.$SCENARIO
#
echo "--------------------------------------------------"
echo "    Running PRESHP for $SCENARIO"
echo "--------------------------------------------------"
#
$EXEC/preshp/preshp << IEOF
USERIN file        :../inputs/userin.hg_bpa.shipping
Input shipping file:../data/hg+bpa_lcp_ships.fy2005a.preshp
Output Messages    :../msg/msg.preshp.$SCENARIO
Output EMBR        :../embr/embr.preshp.$SCENARIO
EMAR error file    :../error/error.preshp.$SCENARIO
IEOF
```

Exhibit 3-19. Example of a PRESHP job script.

3.6 CNTLEM

The CNTLEM (**Co**NT**ro**L **EM**issions) module allows the user to simulate the effects of various control strategies on the emissions contained in the inventory. This module provides the user with methods for

Projecting (or backcasting) a base year emission inventory to represent emissions levels for another year, based on user-specified projection factors for changes in activity levels by source category,

Assessing and comparing the effects on emissions levels (and consequently air quality) of different control strategies under consideration.

CNTLEM may be executed at any stage of processing, but it is recommended as the first step after the input inventory has been loaded into EMBR format (i.e., immediately after running PREPNT, PREAM, LBASE or PREFIR). If the input EMBR file has been chemically speciated (using the CHMSPL or SPCEMS modules), CNTLEM will apply control and projection factors to the appropriate chemical mechanism compound based on the criteria pollutant species from which each chemical mechanism compound was derived. In addition, since the CNTLEM module reads and writes an EMBR file, it can be run multiple times on the same inventory. This is usually done to correctly apply multiple control strategies, without the burden of having to calculate a single control factor that reflects the cumulative affect of the various layers. In addition, multiple runs allows for direct QA and reporting of each control strategy.

Projection Factors

Projection factors represent estimated changes in emission levels between the base inventory and projected years. Factors for point sources and area/mobile sources are submitted to CNTLEM through two control factor packets: /PROJECT PTS/ and /PROJECT AMS/. If the input EMBR file has been chemically speciated, CNTLEM applies the projection factor for each chemical mechanism compound. Projection factors for point sources are designated by either the first two digits of the SIC code, the full 4-digit SIC code or by full SCC code. An optional subregion code can be used to further specify the application of the point source factor. AMS projection factors are assigned using the best match criteria (see Section 2.5). Projection factors are applied to all time intervals in the EMBR file. The projection factors in these packets are applied to all pollutants in the inventory. That is, projection factors are not pollutant specific.

Source Category and Source-Specific Controls

CNTLEM also supports the application of controls for individual sources or by source category. These factors can vary by pollutant. For each control to be implemented, the user must supply source identification fields and a control factor for each criteria pollutant. The order of the factors must be consistent with the order of the pollutants listed in the /CRITERIA POLLUTANT/ packet of the USERIN file. Factors can be applied by county, subregion, facility, stack, point, SIC, SCC, and by time interval. The best match criteria is supported between the different parameters (FIPS, facility, stack, plant, SCC) but is not supported in the breakdown within the SCC. The SCC must be an exact match or blank.

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ENVIRON

FIPS State/County Code Controls

State and county FIPS code controls are used to apply factors to all sources within an entire county. The order of the criteria pollutant factors is the same order as listed in the /CRITERIA POLLUTANT/ packet. A factor must be provided for each pollutant, (i.e., non-adjusted pollutants are assigned a factor of 1.0.) If the input EMBR file has been chemically speciated, CNTLEM applies a factor to each chemical mechanism compound, using the criteria pollutant that was used to create the chemical mechanism compound. For example, CNTLEM will use the factor for NOx to adjust the emissions for the NO and NO2 species. Factors may be specified by time interval where a blank interval indicates an entire day.

Input Files

The CNTLEM module requires three input files: (1) the user input file, USERIN, (2) the control factors file, and (3) the input EMBR file.

CNTLEM reads four packets from the USERIN:

/CNTLEM/ This packet (Table 3-12) contains a flag which controls an output table option to produce controlled emission totals for each county. If this flag is not set to "YES" only a table for the entire domain is written (Exhibit 3-20). The second, and optional flag, indicates if an exact match must occur for controls to be applied.

Table 3-12. /CNTLEM/ packet of EPS3 global user input file, USERIN.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	C	Packet identifier - /CNTLEM/
2		1-20		Not used
	LPRNTC	21-30	C	Flag which determines if controlled emissions by county are written to message file: YES or NO
3		1-20		Not used
	LEXACT	21-30	C	Flag which determines if an exact match must occur for controls to be applied: YES or NO (default)
4	KEYEND	1-20	C	Packet terminator - /END/

```
/CNTLEM/
Print County Tables: NO
/END/
```

Exhibit 3-20. CNTLEM packet of USERIN.

/COUNTY/ This packet contains the list of counties within the modeling domain (Table 2-8). CNTLEM reads this packet to check if a FIPS county code is valid for the modeling region.

/CRITERIA TABLES/ This packet (Table 2-11) specifies which criteria pollutant output tables, if any, the user wants to include in the output message file. See Section 2.4 for a full discussion on the output tables.

S:\eps3\userguide\EPS3UG-Sec3_CORE.doc   3-41

/SPECIES TABLES/ This packet (Table 2-11) specifies which chemical mechanism compound output tables, if any, the user wants to include in the output message file.   See Section 2.4 for a full discussion on the output tables.

The second CNTLEM input file, the control factors file (Exhibit 3-21) also consists of a series of packets. This file may contain four packets (all of which are optional), are described below.

/PROJECT PTS/ This packet (Table 3-13) contains projection factors for estimating the effects of changes in activity levels between base and projection years for point sources. There is one factor for all pollutants. The factor is applied by two digit SIC, four digit SIC or by SCC code. Best-match criteria is supported.

Table 3-13. /PROJECT PTS/ packet of EPS3 control factor input file.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	C	Packet identifier - / PROJECT PTS /
2	INFIPS	1-5-		FIPS county code
	INSBRG	7-11	C	Subregion (optional)
	INSIC	13-22	C	SIC or SCC code
	GFACIN	24-33	R	One projection factor for all pollutants
3	KEYEND	1-20	C	Packet terminator - /END/

/PROJECT AMS/ This packet (Table 3-14) contains the projection factors for estimating the effects of changes in activity levels between base and projection years for area and mobile sources. Each record consists of a FIPS code, the first four digits or full ASC code, and the projection factor. Best-match criteria is supported.

Table 3-14. /PROJECT AMS/ packet of EPS3 control factor input file.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	C	Packet identifier - / PROJECT AMS /
2	INFIPS	1-5-		FIPS county code
	INSBRG	7-11	C	Subregion (optional)
	INSCC	13-22	C	SCC code
	GFACIN	24-33	R	One projection factor for all pollutants
3	KEYEND	1-20	C	Packet terminator - /END/

/FIPS CODE/ This packet (Table 3-15) contains factors for applying controls to all sources in a given county. Each record consists of a FIPS code, as well as the time interval for which the controls apply. The beginning and ending hour fields can be left blank, indicating that the controls are to be applied throughout the entire inventory episode. The final data fields contain the control factors. There is one factor for each pollutant in the /CRITERIA POLLUTANT/ packet, in the same order as specified as the packet.

Table 3-15. /FIPS/ packet of EPS3 control factor input file.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	C	Packet identifier - /FIPS/
2	INFIPS	1-5		FIPS county code
	INSBRG	7-11	C	Subregion (optional)
	IHBEG	12-16	I	Beginning hour to apply factor (optional)
	IHEND	17-21	I	Ending hour to apply factor (optional)
	FACIN(1)	22-31	R	Control factor for 1st criteria pollutants
	…FACIN(10)	…121-130		(allow 10 spaces for each factor
3	KEYEND	1-20	C	Packet terminator - /END/

/SOURCE CATEGORY/ This packet (Table 3-16) allows the user the greatest flexibility to specify controls. The controls can be applied by FIPS code, subregion code, facility, stack, point id, SIC, source category code and/or time interval. This is the area where the best match criteria can be utilized to the greatest degree. By using global codes for the wide-sweeping controls, and exact codes for controls that are specific to a few sources, the user can implement a complicated control strategy with a minimal number of control factor records. Each data record in the packet contains control factors for each criteria pollutant, in the order of the /CRITERIA POLLUTANT/ packet. Note however, that the SCC must be an exact match or a global match, it is not broken into subcomponents for this best match criteria.

Table 3-16. /SOURCE CATEGORY/ packet of EPS3 control factor input file.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	C	Packet identifier - /SOURCE CATEGORY/
2	INFIPS	1-5		FIPS county code
	INSBRG	7-11	C	Subregion
	INPLT	13-22	C	Facility ID
	INSTK	24-33	C	Stack ID
	INPNT	35-44	C	Point ID
	INSIC	46-69	C	SIC code
	INSCC	51-60	C	SCC code
	IHBEG	62-66	I	Beginning hour to apply factor
	IHEND	67-71	I	Ending hour to apply factor
	FACIN(1)	72-81	R	Control factor for 1st criteria pollutants
	…FACIN(10)	…162-171		(allow 10 spaces for each factor
3	KEYEND	1-20	A	Packet terminator - /END/

```
/FIPS CODE/
48000          -9   -9      0.9      1.0      1.0
48039          -9   -9      0.9      0.5      0.9
/END/

/SOURCE CATEGORY/
00000                                      2102004000   -9   -9      1.0
     0.5       1.0
48001                                      2103000000   -9   -9      1.0
     0.5       1.0
48505          0003       1      006                   08   16      0.0
     0.0       0.0
/END/

/PROJECT AMS/
00000     2102000000      1.12
48000     2310001000      1.09
/END/

/PROJECT PTS/
00000          4911      1.54
/END/
```

Exhibit 3-21. Example of a control factors file input to CNTLEM.

Output Files

CNTLEM produces two output files. The first of these, the CNTLEM message file (Exhibit 3-22), consists of several sections. The first section summarizes input and output file names and user options. Unlike the other modules, the CNTLEM message file will always contain a table specific to CNTLEM, regardless of the options specified in the /CRITERIA TABLES/ packet. This output table will provide the user with information on which controls have been applied and the effected changes. In addition, CNTLEM supports all of the output tables governed by the USERIN packets /CRITERIA TABLES/ and /SPECIES TABLES/.

The final output file produced by the CNTLEM module is an EMBR emissions file (Table 2-14) containing the controlled emissions levels.

Exhibit 3-23 shows an example of a CNTLEM job script.

```
                  EPS3 CNTLEM module v. 1.01 Oct 2004      07/25/07 18:41:32


          Input Files
        USERIN file                    :../inputs/userin.test_problem
        Input EMBR file                :../embr/embr.pream.test_problem
        Control factors file           :../inputs/control.factors.area.test_problem


          Output Files
        Output EMBR file               :../embr/embr.cntlem.ar.test_problem


                  EPS3 CNTLEM module v. 1.01 Oct 2004      07/25/07 18:41:32


        Number of counties:   213
        County and total control tables will be created.

 Control factors records read from /PROJECT PTS/ packet:    1 with     1 unique controls
 Control factors records read from /PROJECT AMS/ packet:    2 with     2 unique controls
 Control factors records read from /SOURCE CATEGORY/ packet:    3 with      3 unique controls.
 Control factors records read from /FIPS CODE/ packet:   2 with   2 unique controls.

 Total Emissions Processed
                 English Tons

                       NOX          CO         VOC
        -----------------------------------------------------------
        Input Emissions     647.1180   1006.4943   1826.7257
        Output Emissions    585.8311    979.4699   1825.9321
        Emissions Skipped        0.          0.          0.
        -----------------------------------------------------------



                         Totals by Source Category for Entire Domain
                   P A F
                   R S I
                   O C P           NOX                    CO                    VOC
         SIC    SCC    J  S      IN        OUT        IN        OUT        IN        OUT
        -----------------------------------------------------------------------------------------
         2102 2102004000  X X X   14.9035    15.0227     3.6380     2.0093     0.0800     0.0896
         2102 2102005000  X   X    2.3720     2.3910     0.1507     0.1688     0.         0.
         2102 2102006000  X   X    4.0167     4.0488     2.9716     3.3170     0.0700     0.0784
         2102 2102007000  X   X    1.1421     1.1512     0.2904     0.3196     0.0200     0.0224
         2103 2103004000      X    1.6787     1.5108     0.3915     0.3865     0.0200     0.0200
         2103 2103005000      X    0.1700     0.1530     1.4400     1.3750     0.         0.
```

Exhibit 3-22. Example of CNTLEM message file.

```
#!/bin/csh
#
#    --- Sample job script for running the
#        EPS3 module CNTLEM
#
set EXEC = /models/eps3/src
#
set SCENARIO = test_problem
#
rm -f ../msg/msg.cntlem.ar.$SCENARIO
rm -f ../embr/embr.cntlem.ar.$SCENARIO
#
#
echo "---------------------------------------------------"
echo "    Running CNTLEM for $SCENARIO - area sources"
echo "---------------------------------------------------"
#
$EXEC/cntlem/cntlem << IEOF
USERIN file        :../inputs/userin.$SCENARIO
Input EMBR file    :../embr/embr.pream.$SCENARIO
Control factors    :../inputs/control.factors.area.$SCENARIO
Output Messages    :../msg/msg.cntlem.ar.$SCENARIO
Output EMBR file   :../embr/embr.cntlem.ar.$SCENARIO
IEOF
```

Exhibit 3-23. Example of a CNTLEM job script.

3.7 CHMSPL

The CHMSPL (**CH**e**M**ical **SPL**it) module allows the user to introduce the degree of chemical resolution required for air quality modeling. The primary functions of CHMSPL are

To disaggregate criteria pollutant emissions into the chemical species used in the chemical mechanism employed by the CAM_X, and

To create a chemically speciated EMBR file.

> ➢ **Note**
> As of the Spring of 2008 an additional chemical speciation module has been developed in EPS3. The new module, SPCEMS, is described in Section 3.7. Review both CHMSPL and SPCEMS to determine the appropriate module for your application.

CHMSPL uses both default split factors and speciation profiles to convert emissions from criteria pollutants into the chemical compounds, or model-ready species. All chemical split information must be provided by the user. In order for CHMSPL to create a species, that species/compound must be listed in either the /DEFAULT SPLITS/ packet or the splits factor file. The /DEFAULT SPLITS/ packet of the USERIN provides the default chemical splits for those pollutants whose splits are not source dependent (e.g. NOx, CO). The speciation profiles provide the split factors to generate the chemical mechanism compounds for air quality modeling.

A speciation profile is a broader category than a source category. Typically, a speciation profile is defined by the fuel being burned during the process that produces the emissions. Therefore, many source categories can be lumped under the same speciation profile, provided they all burn the same fuel. CHMSPL assigns a speciation profile code based on the SCC code on the EMBR record; the speciation profile code determines the "split factors" for that particular profile. The split factors are multiplicative factors for converting grams of criteria pollutant emissions into moles of chemical mechanism compound.

The user controls which species/compounds are generated for the modeling application through the USERIN /SPECIES LIST/ packet. Table 3-17 lists the species/compounds for a typical ozone application employing the Carbon Bond IV mechanism. Refer to Section 4.2, describing the EMSCVT utility, for a more detailed discussion of the available options for specifying species.

Table 3-17. Species, with molecular weights (grams per mole) for unit conversion, for typical ozone application with CBIV.

Model Species	Species Name	Molecular Weight[a]
NO[†]	Nitric oxide	30
NO2[†]	Nitrogen dioxide	46
CO[†]	Carbon monoxide	28
SO2[†]	Sulfur dioxide	64
OLE	Olefinic carbon bond (C=C)	32
PAR	Paraffinic carbon bond (C—C)	16
TOL	Toluene (C_6H_5—CH_3)	112
XYL	Xylene (C_6H_6—$(CH_3)_2$)	128
FORM	Formaldehyde (CH_2=O)	16
ALD2	High molecular weight aldehydes (RCHO, R≠H)	32
ETH	Ethene (CH_2=CH_2)	32
MEOH	Methanol (optional)	16
ETOH	Ethanol (optional)	32
ISOP	Isoprene	80

[a]Default Molecular weights for chemical mechanism compounds are provided by the user in the /SPECIES LIST/ packet.
[†]Splits are provided through /DEFAULT SPLITS/ packet of USERIN.

The CHMSPL module compares the chemical mechanism species list in the input split factor file to the list in the /SPECIES LIST/ packet of the USERIN file. When a discrepancy exists between the two lists CHMSPL addresses the inconsistency in the following manner. If a requested species is not in the split factor file and not in the /DEFAULT SPLITS/ packet, CHMSPL will terminate execution with an appropriate message. If the /SPECIES LIST/ packet contains fewer species than contained in the split factor file, a potential error (e.g., loss of mass) may be incorporated into the final inventory, particularly if the missing species is derived from chemical speciation of VOC. Under default conditions, CHMSPL will terminate execution, allowing the user to correct either the species list in the USERIN file or the species included in the split factors file. However, the user has the option of setting an 'override' flag in the /CHMSPL/ packet of the USERIN indicating to use the existing split factor values with the fewer user-specified list of species. This may occur, for example, if the splits factor file includes NASN (not assigned) which is not needed for modeling.

Prior to processing by CHMSPL, the modeling species list in the header records of the EMBR

file will be blank.   If CHMSPL reads an EMBR file in which these fields have been filled, the program terminates without further action; it assumes the file is already speciated. If an input emissions record contains a source that cannot be cross-referenced to a profile code, the record is written to the output error file for review and reprocessing.

Input Files

The CHMSPL program requires four input files: the USERIN file, the pre-speciated EMBR file, the SCC(ASC)/speciation profiles cross-reference file, and the chemical mechanism split factors file.

CHMSPL reads six packets of the USERIN file:

/CHMSPL/   The /CHMSPL/ packet of the USERIN input file contains three option flags (Table 3-18). The first option, the "Use Non-matching lists" flag, indicates if the /SPECIES LIST/ in the USERIN must match the species list in the split factors file for those pollutants not in the /DEFAULT SPLITS/ packet of the USERIN. If the species list provided by the user in the /SPECIES LIST/ packet does not match the species list included in the split factors file a "YES" flag signals CHMSPL to continue processing despite inconsistencies; a "NO" indicates that CHMSPL should stop execution. The second flag, "Print Profile Table", determines if CHMSPL will produce a table of emissions totals by profile code. The third option; "Force Profile Match", determines how CHMSPL treats records without a matching profile code: "YES" indicates that only records for which CHMSPL can determine a profile code will be processed; a "NO" results in speciation of emissions for that record according to the default profile, which is the EPA overall industry average profile (EPA VOC speciation profile " 0000"). See Exhibit 3-24 for an example of this packet.

Table 3-18. /CHMSPL/ packet of EPS3 global user input file, USERIN.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	C	Packet identifier - /CHMSPL/
2		1-20		Not used
	LOVRID	21-30	C	Option which determines if execution continues if species lists are incompatible YES = use incompatible species lists NO = terminate if species lists do not match
3		1-20		Not used
	LPRTPF	21-30	C	Option to print tables by profile code: YES = print tables by profile code NO = do not print profile table
4		1-20		Not used
	LREQPF	21-30	C	Option whether or not to use default profile YES = must have profile code in splits file NO = will look for default profile code
5	KEYEND	1-20	C	Packet terminator - /END/

```
/CHMSPL/
Use Non-match Specs: YES
Print Profile Table: YES
Force Profile Match: YES
/END/
```

Exhibit 3-24. CHMSPL packet of USERIN.

/SPECIES LIST/ This packet (Table 2-11) provides the species list for air quality modeling.

/DEFAULT SPLITS/ This packet defines default split factors for those pollutants whose speciation is not source category dependent (e.g., CO or NOX.) The user provides a value which is applied to the criteria pollutant to estimate the air quality model species. See Exhibit 3-25 for an example packet. The format of this table is shown in Table 3-19. The name of the criteria pollutant must match one of the names in the /CRITERIA POLLUTANT/ packet. The "splits factor" is the percentage of the criteria pollutant that is allocated to the specified air quality modeling species. For example, using the packet below, EPS3 will allocate NOX emissions to 90% NO and 10% NO2. Although this packet could be used for any criteria pollutant, it is not recommended that it be used for hydrocarbons. The chemical makeup of hydrocarbons varies greatly based on the type of source (i.e. the fuel being burned and/or the process being performed), a default split factor will likely result in an inaccurate modeling inventory.

Table 3-19. /DEFAULT SPLITS/ packet of USERIN file.

Line	Columns	Type	Description
1	1-20	C	Packet identifier - /DEFAULT SPLITS/
2+	1-20	C	Label (ignored)
	21-30	C	Name of air quality modeling species
	31-40	C	Parent criteria pollutant name
	41-50	R	Split factor (percent)
3	1-20	C	Packet terminator - /END/

```
/DEFAULT SPLITS/
Nitrous Oxides     : NO        NOX       90
Nitrous Oxides     : NO2       NOX       10
Carbon Monoxide    : CO        CO        100
/END/
```

Exhibit 3-25. /DEFAULT SPLITS/ packet of the USERIN file.

/COUNTY/ This packet (Table 2-8) is read to allow the module to check if a FIPS county code is valid for the modeling region.

/CRITERIA TABLES/ This packet (Table 2-11) specifies which criteria pollutant output tables, if any, the user wants to include in the output message file. See Section 2.4 for a full discussion on the output tables.

/SPECIES TABLES/ This packet (Table 2-11) specifies which chemical mechanism compound output tables, if any, the user wants to include in the output message file. See Section 2.4 for a full discussion on the output tables.

The second input, the EMBR file, can be of any type (AREA, MOBILE, POINT, or COMBINED) and can represent an inventory at any stage of EPS3 processing.
The third input file, the SCC(ASC)/speciation profile cross reference file, provides a list of FIPS codes, facility identification codes, and SCC(ASC) codes along with the code of the speciation profile which most accurately represents the source (Table 3-20). This file is essentially a lookup table that assigns an appropriate speciation profile to each source category code. Although a default version of this file is provided with the EPS3 distribution, the user can use the EMSCVT utility to update the file with any application specific information. The best match criteria is supported. In the standard EPA speciation profile cross reference file, the FIPS and facility identification code fields will contain global values (zeros for FIPS and blanks for facility identification fields), indicating that the profile is to be applied globally to any source matching the SCC(ASC) code. The user may specify state-, county-, facility-, or source-specific speciation profiles by specifying non-zero or non-blank values for the appropriate fields. Exhibit 3-26 is an example of the cross reference file; the last line is an example of a point specific profile code. For each EMBR record, CHMSPL will select the speciation profile with the closest match for the identification code fields.

```
00000                        49000299  9047
00000                        49000399  9047
00000                        49000499  9047
00000                        49000599  9047
00000                        49099998  9047
00000                        49099999  9047
00000                      2461100000  9047
00000                      2461160000  9047
00000                      2461200000  9047
00000                      2461900000  9047
00000                        30182004  9004
00000                        30182005  9004
00000                        30182006  9004
00000                        30182007  9004
48505       0003        1    20200202  LOBO
```

Exhibit 3-26. Example of chemical speciation cross reference file read by CHMSPL.

Table 3-20. SCC(ASC)/speciation profile cross-reference file created by the EMSCVT utility.

Line	Variable	Columns	Type	Description
1+	FIPXRF	1-5	C	FIPS code of state/county: 00000 = applies to all counties in region *nn*000 = applies to all counties in state *nn* *nnmmm* = applies to county *mmm* in state *nn*
	FACXRF	7-16	C	AFS plant identification code (blank = applies to all plants in county)
	STXRF	18-27	I	AFS stack identification code (blank = applies to all stacks in facility)
	CCXRF	29-38	C	Source Classification Code (SCC)/ Area Source Category code (ASC)
	RFXRF	40-44	C	Profile code

> ➤ **Processing Tip**
> To create a source specific speciation profile code, the user may define a five character code. This code must not already exist in the list of profile codes. The standard EPA profile codes have a blank character followed by four digits, while the source specific speciation codes can contain any alphanumeric characters but can have no imbedded blank characters.

The split factors file (Table 3-21), which the user can create with the EMSCVT utility, contains the carbon bond species split factors for each profile code found in the SCC(ASC)/speciation profiles cross-reference file. The first 2 lines are header lines and contain a list of compounds, indicating the order of the split factors for each profile (Exhibit 3-27). The data records, one for each speciation profile code, contain the factors that will be used to create the chemical mechanism species from the assigned criteria pollutant.

Table 3-21. Split factors file created by the EMSCVT utility and input into the CHMSPL module.

Line	Variable	Columns	Type	Description
1	NSPLIT	1-5	I	Number of compounds in splits file
2+	SPLNAM(*)	1-10	C	Compund name
	SPLMOL(*)	12-16	R	Molecular weight
	SPLCRT(*)	18-22	C	Criteria pollutant that creates compound
3+	PRFSPL(*)	1-5	C	Profile code (no imbedded blank characters)
	SPLTAB(*)	6-306	R	Splitting factor for compound1
			R	Splitting factor for compound 2
	•			
	•			
	•		R	Splitting factor for compound NSPLIT

> ➤ **Processing Tip**
> The split factors file must also contain any source-specific speciation profiles created by the user. To incorporate a source specific speciation profile: 1) create a unique profile code, 2) calculate the split factors (conversion from grams to moles) 3) add a line to the split factors containing the profile code as the first field and the split factors as the remaining fields.

```
12
OLE          32.0 VOC
PAR          16.0 VOC
TOL         112.0 VOC
XYL         128.0 VOC
FORM         16.0 VOC
ALD2         32.0 VOC
ETH          32.0 VOC
MEOH         16.0 VOC
ETOH         32.0 VOC
ISOP         80.0 VOC
NR           16.0 VOC
NASN          1.0 VOC
0000  0.178E-02 0.238E-01 0.628E-03 0.374E-03 0.527E-03 0.121E-02 0.112E-02 0.439E-03 0.304E-03 0.587E-04 0.124E-01 0.850E-02
0001  0.000E+00 0.276E-01 0.000E+00 0.000E+00 0.140E-01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.679E-02 0.000E+00
0002  0.000E+00 0.349E-01 0.000E+00 0.000E+00 0.162E-01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.663E-03 0.000E+00
0003  0.000E+00 0.202E-01 0.217E-03 0.000E+00 0.266E-02 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.385E-01 0.000E+00
0004  0.416E-02 0.323E-01 0.000E+00 0.000E+00 0.253E-02 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.222E-01 0.000E+00
0005  0.713E-04 0.147E-02 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.417E-02 0.000E+00 0.000E+00 0.000E+00 0.540E-01 0.000E+00
0007  0.000E+00 0.436E-03 0.000E+00 0.000E+00 0.999E-02 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.432E-01 0.000E+00
```

Exhibit 3-27. Example of split factors file input to CHMSPL.

Output Files

CHMSPL produces three output files; Exhibit 3-28 shows an example of a CHMSPL job script. The first of these is a message file containing the output tables requested by the user in the /CRITERIA TABLES/ and /SPECIES TABLES/ packets. If the output option for tabulating emissions totals by profile has been selected, the message file will also include these tables. Exhibit 3-29 contains a sample CHMSPL message file. The first section of the message file is a summary of the input and output file names, the beginning and ending dates and times for the inventory, and the user-specified options from the /CHMSPL/ packet of the USERIN file. The next section provides information regarding the number of species included in the splits file, the number of speciation profiles read by the program, the number of EMBR records processed; this section may also contain a variety of warning messages, indicating conditions which did not halt program execution but of which the user should be aware. This is followed by a tabular summary of input and output emissions totals by county and carbon bond species and the optional tables of output emissions by speciation profile code.

The second file generated by the CHMSPL module is the chemically speciated EMBR file; refer to Table 2-14 for a description of the EMBR format.

Finally, any input records that cannot be processed by the CHMSPL module are output to an EMAR error file. This file will be empty if CHMSPL successfully processes all records. The user may examine this file to determine the appropriate action to remedy any problems.

```
#!/bin/csh
#
#    --- Sample job script for running the
#        EPS3 module CHMSPL
#
set EXEC = /models/eps3/src
#
set SCENARIO = test_problem
#
rm -f ../msg/msg.chmspl.ar.$SCENARIO
rm -f ../embr/embr.chmspl.ar.$SCENARIO
rm -f ../error/emar.chmspl.ar.$SCENARIO
#
echo "----------------------------------------------"
echo "    Running CHMSPL for $SCENARIO - area sources"
echo "----------------------------------------------"
#
$EXEC/chmspl/chmspl << IEOF
USERIN file        :../inputs/userin.$SCENARIO
Input EMBR file    :../embr/embr.cntlem.ar.$SCENARIO
Splits file        :../inputs/splitfac.VOC_to_TOG.std_profiles.cb4.eps3.15jan07
ASC profile XREF   :../inputs/chemical.speciation.xref.cb4.12Dec04
Output Messages    :../msg/msg.chmspl.ar.$SCENARIO
Output EMBR file   :../embr/embr.chmspl.ar.$SCENARIO
EMAR error file    :../error/emar.chmspl.ar.$SCENARIO
IEOF
```

Exhibit 3-28 Example of a CHMSPL job script.

```
                    EPS3 CHMSPL module v. 1.01 Oct 2004

             Input Files
             USERIN file                     :../inputs/userin.test_problem
             Input EMBR file                 :../embr/embr.cntlem.ar.test_problem
             Splits file                     :../inputs/splitfac.VOC_to_TOG.std
                                             :../inputs/chemical.speciation.xref.cb4

             Output Files
             Output EMBR file                :../embr/embr.chmspl.ar.test_problem
             EMAR error file                 :../error/emar.chmspl.ar.test_problem




/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\

WARNING: Cannot find the /SPECIES TABLES/ packet of USERIN file.
Only default tables for speciated pollutants will be written to the message file.

/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\

EPS3 CHMSPL module v. 1.01 Oct 2004       07/25/07 18:41:37

             File note                       :CAMx Modeling of Tx regional, 9/13/99
             Episode date (Calander)         :990913
             Episode date (Julian)           :99256
             Beginning hour                  :    0
             Ending hour                     :   24
             Use inconsistent species lists:YES
             Write totals by profile code   :YES
             Force profile match            :YES

 Number of species in the splits file:      12
 Number of factors read from splits file:     373

 ----------------------------------------------------------------
          Note to the user:  The criteria pollutant emissions are
                             reported as the sum of all contributing
                             speciated emissions.

                             The speciated emissions are reported as
                             methane equivalent.  Therefore the output
                             criteria emissions may not match the input
                             criteria emissions.
 ----------------------------------------------------------------

Total Criteria Emissions Processed
                  English Tons

                          NOX          CO          VOC
 ----------------------------------------------------------
 Input Emissions       585.8311     979.4699     1825.9321
 Output Criteria       585.8311     979.4699     1825.9321
 Output Speciated      585.8311     979.4698     1781.7369
 Emissions Skipped        0.          0.           0.
 Written to EMAR          0.          0.           0.
 ----------------------------------------------------------
```

Exhibit 3-29. Example of a CHMSPL message file.

3.8 SPCEMS

The SPCEMS (**SP**e**C**iate **EM**i**S**sions) module allows the user to generate the degree of chemical resolution required for air quality modeling. The primary functions of SPCEMS are

   To disaggregate criteria pollutant emissions into the chemical species employed by the CAM$_X$ (or other AQ Model),

   To optionally compute new compounds by taking the difference of two inventory criteria pollutants, and

   To create a chemically speciated EMBR file.

The input emission inventory is comprised of compounds or chemical classes such as CO, NOX, VOC, and PM10. However, Air Quality Models use a set of chemical compounds/species, referred to as modeling species, based on a photochemical mechanism (e.g., CBIV, CB05, SAPRC99) to simulate atmospheric chemistry. SPCEMS provides the means to convert the input emission inventory compounds to the required modeling species.

SPCEMS was developed in the spring of 2008 to support chemical speciation for multiple criteria pollutants. The previously used module, CHMSPL, described in section 3.6, was designed specifically to support the speciation of hydrocarbons. SPCEMS allows the speciation of any criteria pollutant and requires that **all** criteria pollutants be speciated through the input speciation factors input file. This is a siginificant difference from CHMSPL which uses the /DEFAULT SPLITS/ packet to speciate those criteria pollutants which are not source dependent (e.g. NOx, CO). SPCEMS does not use the /DEFAULT SPLITS/ packet, each criteria pollutant must be explicity defined in the input speciation factors file.

> ➢ **Note**
> The input emission inventory to SPCEMS must be pre-speciated.
> You may **not** run CHMSPL to generate one set of species and
> then run SPCEMS to generate another set. Either run CHMSPL or
> run SPCEMS; not both.

The input speciation factors are defined as a 'speciation profile'. Typically, a speciation profile is defined by the fuel being burned during the process that produces the emissions. A speciation profile is a broader category than a source category. Therefore, many source categories can be lumped under the same speciation profile, provided they all burn the same fuel. The speciation profile is assigned to the inventory's sources using a speciation cross-reference based on state/county FIPS code, SCC, and criteria pollutant for non-point sources. The speciation profile code determines the speciation factors that are applied to that source. The factors convert grams of criteria pollutant emissions into moles of modeling species. The exception is particulates which are mass based.

> ➢ **Note**
> Best match criteria is applied to the speciation cross-reference
> lookup. For area, on-road, and non-road sources this includes
> FIPS, ASC and pollutant. For point sources it includes FIPS, plant,
> stack, point, SCC and pollutant.

Speciation of Hydrocarbons

When speciating hydrocarbons you must know what is reported in the inventory and what the speciation profiles represent. For inventories with criteria pollutant VOC, an additional factor may be needed to convert the VOC mass to TOG mass if the speciation profiles are computed based on TOG. This is the most common practice. The TOG profiles are used (instead of VOC profiles) since some of the TOG mass gets assigned to model species. Using VOC-only profiles would underestimate the mass being emitted. The /SPCEMS/ packet allows the user to indicate which input criteria pollutant, if any, is to be converted and the name of the converted compound. In addition, an input conversion factor file must be specified which provides the conversion factors by profile code.

Through the speciation profiles SPCEMS converts emissions from criteria pollutants into the modeling species. The output modeling species are defined through the /SPECIES LIST/ packet of the USERIN. If a speciation profile includes a model species that is not specified in the /SPECIES LIST/ packet then it is excluded from modeling, this may result in a loss of mass. An example is a profile with a component of 'UNK' (unknown) that may not be included in the /SPECIES LIST/ packet. Exhibit 3-30 is an example of the /SPECIES LIST/ packet that includes CB05 and particulates.

Prior to running SPCEMS, the modeling species list in the header records of the input EMBR file will be blank. If SPCEMS reads an EMBR file in which these fields have been filled, the program terminates without further action; it assumes the file is already speciated.

If an input emissions record contains a source that cannot be cross-referenced to a profile code, the record is written to the output error file for review and/or reprocessing. If a profile code is assigned to a source but the speciation factors for that profile are not defined then the record is written to the output error file for review and/or reprocessing.

```
This packet defines the species list that will be generated in the
modeling inventory.  The species name, associated criteria pollutant, and
molecular weight of the species are required. Only species in this list
will be included in the output inventory.
The fields are:
 1-20 label (ignored)
21-30 species name
31-40 name of assiciated criteria pollutant
41-50 molecular weight

/SPECIES LIST/
                  :NO          NOX          46.0
                  :NO2         NOX          46.0
                  :OLE         VOC          32.0
                  :PAR         VOC          16.0
                  :TOL         VOC         112.0
                  :XYL         VOC         128.0
                  :FORM        VOC          16.0
                  :ALD2        VOC          32.0
                  :ETH         VOC          32.0
                  :MEOH        VOC          16.0
                  :ETOH        VOC          32.0
                  :ISOP        VOC          80.0
                  :ETHA        VOC          32.0
                  :IOLE        VOC          64.0
                  :TERP        VOC         160.0
                  :ALDX        VOC          32.0
                  :CH4         VOC          16.0
                  :NR          VOC          16.0
                  :NASN        VOC           1.0
                  :CO          CO           28.0
                  :SO2         SO2          64.0
                  :NH3         NH3          17.0
                  :PSO4        SO4           1.0
                  :PMC         PM10          1.0
                  :FPRM        PM2_5         1.0
                  :PEC         PM2_5         1.0
                  :PNO3        PM2_5         1.0
                  :POC         PM2_5         1.0
/END/
```

Exhibit 3-30. Example of /SPECIES LIST/ packet of CB05 and particulates.

Particulates

In addition to generating output model species based on speciation profiles via the cross-reference information SPCEMS also has the ability to generate output model species by taking the difference of two criteria pollutants. This option is specifically provided to support the calculation of PM coarse. An emission inventory often provides estimated emissions for PM10 (10 microns or less) and PM2_5 (2.5 microns or less). If both PM10 and PM2_5 are included in modeling then the fine (2.5 or less) component is double counted.

SPCEMS, through the /SPCEMS/ packet described below, provides a mechanism to remove the fine component from the larger component. An example, PMC = PM10 – PM2_5. The computed

computed species must exist in the /SPECIES LIST/ packet (PMC in the example). And both PM10 and PM2_5 must be criteria pollutants defined in the input EMBR file. If the difference results in a negative value then the result is set to zero. The computed output model species, PMC in the example, will not be speciated via the cross-reference/profile lookups and the computed output can not be used in a second difference calculation. The PM10 criteria pollutant will be carried through the EPS3 modeling and included in report tables; it represents the PM10 not PMC.

The emissions generated by taking a difference are not reported in the optional output profile tables. This is because there is no profile code associated with these emissions.

Input Files

The SPCEMS program reads five input files: the USERIN file, the pre-speciated EMBR file, the SCC(ASC)/speciation profiles cross-reference file by criteria pollutant, the chemical speciation factors file, and optionally, a conversion factors file.

SPCEMS reads five packets of the USERIN file:

/SPCEMS/ packet, described below, provides the required parameters of the module.

/SPECIES LIST/ packet (Table 2-11) provides the species list for air quality modeling.

/COUNTY/ packet (Table 2-8) is read to allow the module to check if a FIPS county code is valid for the modeling region. Any counties not found in this packet will be dropped.

/CRITERIA TABLES/ packet (Table 2-12) specifies which criteria pollutant output tables, if any, the user wants to include in the output message file. See Section 2.4 for a full discussion on the output tables.

/SPECIES TABLES/ packet (Table 2-12) specifies which speciated compound output tables, if any, the user wants to include in the output message file. See Section 2.4 for a full discussion on the output tables.

The /SPCEMS/ packet is the driver for this module. The first line following the /SPCEMS/ packet header (Table 3-22) is the flag, "Print Profile Table", which determines if SPCEMS will include tables of emissions totals by profile code in the output message file. It is highly recommended that this option always be specified as YES. The next option; "Force Profile Match", determines how SPCEMS treats records without a matching profile code: "YES" indicates that only records for which a profile code match is found will be processed; a "NO" results in assigning a default profile code "0000" if the cross-reference profile code is not found in the speciation factors file.

The next record indicates if conversion factors should be applied to hydrocarbons. If the record is blank then no conversion factors will be applied. If conversion is required then specify the "from" criteria pollutant name followed by the "to" pollutant name. For example, "VOC TOG" means that the input criteria pollutant labeled VOC should be converted to TOG prior to applying

applying speciation factors. If specified, the "from" pollutant must exist in the criteria pollutant list on the EMBR header. The pollutant names must match those specified in the conversion factors file discussed below.

The following optional /SPCEMS/ packet record(s) specify new output modeling species generated by subtracting one criteria pollutant from another. The format of the line is "NewName = CriteriaA – CriteriaB", for example, PMC = PM10 – PM25. Multiple compounds may be computed, each specified on a separate line. SPCEMS will continue to read until the /END/ terminator is read. See Exhibit 3-31 for an example of this packet.

Table 3-22. /SPCEMS/ packet of EPS3 global user input file, USERIN.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	C	Packet identifier - /SPCEMS/
2		1-20		Not used
	LPRTPF	21-30	C	Option to print tables by profile code: YES = print tables by profile code NO = do not print profile table
3		1-20		Not used
	LREQPF	21-30	C	Option whether or not to use default profile 0000 YES = must specify profile in xref NO = will look for default profile code
4		1-20		Not used
	FROMCRT	*	C	Name of the criteria pollutant if converting from one compound to another (e.g. VOC)
	TOCRT	*	C	Name of the pollutant converting to (e.g. THC)
5+		1-20		Not used
		21-	C	String to specify when computing a new compound from two existing criteria pollutants. Format : NewName = CName - BName
6	KEYEND	1-20	C	Packet terminator - /END/

```
/SPCEMS/
PRINT PROFILE TABLE: YES
FORCE PROFILE MATCH: YES
Apply CONV Factors : VOC TOG
Calc Particulate   : PMC = PM10 – PM2_5
/END/
```

Exhibit 3-31. Example of /SPCEMS/ packet of USERIN.

The second input, the EMBR file, can be of any type (AREA, MOBILE, POINTS, or FIRPTS) and can represent an inventory at any stage of EPS3 processing.

The SCC(ASC)/speciation profile cross reference file provides a list of FIPS code, facility identification, SCC(ASC) code and criteria pollutant name indicating the speciation profile code which most accurately represents the source (Table 3-23). This file is essentially a lookup table that assigns an appropriate speciation profile to each source category code and criteria pollutant.

Table 3-23. SCC(ASC)/speciation profile cross-reference file.

Line	Variable	Columns	Type	Description
1+	FIPXRF	1-5	C	FIPS code of state/county: 00000 = applies to all counties in region *nn*000 = applies to all counties in state *nn* *nnmmm* = applies to county *mmm* in state *nn*
	FACXRF	7-16	C	AFS plant identification code (blank = applies to all plants in county)
	ISTXRF	18-27	I	AFS stack identification code (blank = applies to all stacks in facility)
	SCCXRF	29-38	C	Source Classification Code (SCC)/ Area Source Category code (ASC)
	PRFXRF	40-45	C	Profile code
	CRTXRF	47-57	C	Criteria pollutant name

The best-match specification is supported. In the EPS3 default speciation profile cross reference file, the FIPS and facility identification code fields will contain global values (zeros for FIPS and blanks for facility identification fields), indicating that the profile is to be applied globally to any source matching the SCC(ASC) code and pollutant. The user may specify state-, county-, facility-, or source-specific speciation profiles by specifying non-zero or non-blank values for the appropriate fields. Exhibit 3-32 is an example of the cross reference file; the first two lines indicate that CO and NOX will be mapped to the default profile 0000. The third line indicates that all MV source categories will use profile 92000 to speciate PM2_5. The remaining lines indicate VOC profiles for exact match SCC codes. For each criteria pollutant on an EMBR record, SPCEMS will select the speciation profile with the closest match for the identification code fields. If no match is found for any of the criteria pollutants on a record the entire record is written to the error file.

> ➢ **Note**
> If converting from one hydrocarbon to another, for example VOC to TOG, the cross-reference file must contain pollutant codes for the 'from' pollutant. That is, the cross-reference file must contain records for the criteria pollutants specified in the EMBR header.

```
00000                         0000000000  0000  CO
00000                         0000000000   0000  NOX
00000                         MV00000000 92000  PM2_5
00000                         MV01230EXH H2KWT  VOC
00000                         MV01230EVP H2KGV  VOC
00000                         MV01250EXH H2KWT  VOC
00000                         MV01250EVP H2KGV  VOC
00000                         MV01270EXH H2KWT  VOC
00000                         MV01270EVP H2KGV  VOC
```
Exhibit 3-32. Example of chemical speciation cross reference file read by SPCEMS.

> ➤ **Processing Tip**
> To create a source specific speciation profile, define a character
> code that does not exist in the list of profile codes. The standard
> EPA profile codes for VOCs have a blank character followed by four
> digits the standard particulate profiles are 5 digits beginning with '9'.
> Source specific speciation codes can contain any alphanumeric
> characters but can have no imbedded blank characters.

The speciation factors file format is provided in Table 3-24. This file format corresponds to the output file format from EPA's Speciation Tool (Exhibit 3-33). Unlike most EPS3 input files which are fixed format files this file is a 'free' format, each field is separated by one or more spaces. Any records that have a '#' character in the first column, or any blank lines, will be skipped.

The data records specify the speciation profile code, the criteria pollutant name to be disaggregated, the output model species name, and the factors to compute the output emissions. In general terms,

Output (moles) = Input (grams) * [Split Factor / Divisor] (moles/gram)

Or specifically, using the Exhibit data,

Output NO (moles) = Input NOx (grams) * [.90 / 46.] (moles/gram)

The first factor, the split factor, indicates the fraction of the inventory pollutant that is to be assigned to the model species. The second factor represents molecular weight. In this case the sum of the split factors for a single profile **and** criteria pollutant will typically be 1.0. However, as shown in Exhibit 3.33 with profile D101, a computed speciation factor can be provided as the split factor with a divisor of 1.0. In this case the sum of the factors does not equal 1.0 since they are adjusted by the molecular weights.

It is important to realize that not all air quality models use the same set of modeling species. Therefore, a different speciation factors file may be necessary for emissions modeling. An example is CAMx uses FPRM while CMAQ uses PMFINE. It is imperative that the emissions modeler understand what is required by the air quality model they will be using.

When SPCEMS reads the speciation factors file it only stores the data it will need for computing output emissions. Any records with a criteria pollutant name that is not in the EMBR header or is not the "to" pollutant specified in the /SPCEMS/ packet will be skipped. For example, if you are converting hydrocarbons from VOC to TOG then the speciation factors file must provide factors for TOG. Any records with a speciated compound name not in the /SPECIES LIST/ packet will be skipped. In addition, any records that have a divisor equal to zero, the module will set the divisor to 1.0.

Table 3-24. Speciation factors file input into the SPCEMS module.

Line	Variable	Columns	Type	Description
1+	PRFFAC(*)		C	Profile code (no imbedded blank characters)
	POLTMP		C	Criteria pollutant name
	AQMTMP		C	Speciated compound name
	SPCFAC(*,*,*)		R	Split factor
			R	Divisor
			R	Mass fraction (not used)

```
# File generated via the Speciation Tool at ENVIRON
# 2007 Nov with SPECIATE4.0 data
#
0000  NOX        NO              0.90         46.        0.90
0000  NOX        NO2             0.10         46.        0.10
0000  CO         CO                 1         28.           1
D101    TOG    ALD2          1.96E-04   1.00  1.96E-04
D101    TOG    ALDX          1.80E-06   1.00  1.80E-06
D101    TOG    ETH           2.07E-03   1.00  2.07E-03
D101    TOG    ETHA          4.42E-04   1.00  4.42E-04
D101    TOG    FORM          1.02E-03   1.00  1.02E-03
D101    TOG    IOLE          3.12E-04   1.00  3.12E-04
D101    TOG    ISOP          2.29E-05   1.00  2.29E-05
# the following records represent particulate profiles
92095         PM2_5        FPRM         0.8279       1.0000       0.8279
92095         PM2_5        PEC          0.0170       1.0000       0.0170
92095         PM2_5        PNO3         0.0021       1.0000       0.0021
92095         PM2_5        POC          0.0263       1.0000       0.0263
92095         PM2_5        PSO4         0.1267       1.0000       0.1267
```

Exhibit 3-33. Example of partial speciation factors file input to SPCEMS.

The conversion factors file is an optional input file. This file is required if you are converting input emission inventory pollutants from one hydrocarbon to another. As stated earlier, often an input emissions inventory is reported as VOC while the Speciation Tool generates profiles as TOG. In order to accurately represent the emissions, the VOC estimate is multiplied by a factor to 'add in' the non-reactive portion that is typically not reported. This file is also output by the Speciation Tool and goes hand-in-hand with the speciation factors file. When conversion is required SPCEMS verifies that every 'TOG' speciation profile has a corresponding conversion factor. If it comes across a case that does not match it will display a message and abort execution.

The file format, like the speciation factors file, is a free format. Table 3-25 provides the file specifics. Exhibit 3-34 is an example of this file.

Table 3-25. Conversion factors file input into the SPCEMS module (optional).

Line	Variable	Columns	Type	Description
1+	TMPFRM		C	Name of criteria pollutant converting from
	TMPTO		C	Name of pollutant converting to
	TMPPRF		C	Speciation profile code
	TMPFAC		R	Conversion factor

```
# File generated via the Speciation Tool at ENVIRON
# 2007 Nov with SPECIATE4.0 data
#
VOC          TOG          0001          1.63934426
VOC          TOG          0002          1.00000000
VOC          TOG          0003          2.27272727
VOC          TOG          0004          1.39860140
VOC          TOG          0005          6.80272109
VOC          TOG          0007          3.33333333
VOC          TOG          0008          1.16822430
```
Exhibit 3-34. Example of conversion factors file (VOC to TOG) input to SPCEMS.

Output Files

SPCEMS produces three output files. Exhibit 3-35 shows an example of a SPCEMS job script.
The first output file specified is a message file containing the output tables requested by the user
in the /CRITERIA TABLES/ and /SPECIES TABLES/ packets. If the output option for
tabulating emissions totals by profile has been selected, the message file will also include these
tables. Exhibit 3-36 contains a sample SPCEMS message file. The first section of the message
file is a summary of the input and output file names, the user-specified options from the
/SPCEMS/ packet of the USERIN file, and the list of output modeling specie/compounds
specified in the /SPECIES LIST/ packet. The next section provides information regarding the
number of input records read for each input file. This section may also contain a variety of
warning messages, indicating conditions which did not halt program execution but of which the
user should be aware. This is followed by a tabular summary of input and output emissions
totals. Next will be the emission tables by profile code, if requested, followed by the additional
output tables requested in the /CRITERIA TABLES/ and /SPECIES TABLES/ packets.

The second file generated by the SPCEMS module is the chemically speciated EMBR file; refer
to Table 2-14 for a description of the EMBR format.

Finally, any input records that cannot be processed by the SPCEMS module are output to an
EMAR error file. This file will be empty if SPCEMS successfully processes all records. The
user may examine this file to determine the appropriate action to remedy any problems.

```
#!/bin/csh
#
#   --- Sample job script for running the
#       EPS3 module SPCEMS
#
set EXEC = /models/eps3/src
#
set SCENARIO = testpm
#
rm -f ../msg/msg.spcems.ar.$SCENARIO
rm -f ../embr/embr.spcems.ar.$SCENARIO
rm -f ../error/emar.spcems.ar.$SCENARIO
#
echo "-------------------------------------------------"
echo "    Running SPCEMS for $SCENARIO - area sources"
echo "-------------------------------------------------"
#
$EXEC/spcems/spcems << IEOF
USERIN file         :../inputs/userin.$SCENARIO
Input EMBR file     :../embr/embr.cntlem.ar.$SCENARIO
SpeciationFactors   :../inputs/gspro_CB05_CAMX_26Sep2007_TOG_PM.dat
Profile XREF        :../inputs/speciation.xref.by_criteria.30mar2008
Conversion Factors  :../inputs/gscnv_CB05_CAMX_26Sep2007.dat
Output Messages     :../msg/msg.spcems.ar.$SCENARIO
Output EMBR file    :../embr/embr.spcems.ar.$SCENARIO
EMAR error file     :../error/emar.spcems.ar.$SCENARIO
IEOF
```

Exhibit 3-35 Example of a SPCEMS job script.

```
                   EPS3 SPCEMS module v. 1.00 Apr 2008

            Input Files
     USERIN file                  :../inputs/userin.testpm
     Input EMBR file              :../embr/embr.cntlem.ar.testpm
     Speciation factors file
:../inputs/gspro_CB05_CAMX_26Sep2007_TOG_PM.dat      Cross reference file
  :../inputs/speciation.xref.by_criteria.30mar2008      Conversion factors
file    :../inputs/gscnv_CB05_CAMX_26Sep2007.dat

            Output Files
     Output EMBR file             :../embr/embr.spcems.ar.testpm
     EMAR error file              :../error/emar.spcems.ar.testpm

            EPS3 SPCEMS module v. 1.00 Apr 2008      04/22/08 10:38:01
     Write totals by profile code :YES
     Force profile match          :YES
     Apply conversion factors     :YES
                    From          :VOC
                    To            :TOG
     Calculate new from existing  :YES
                                  PMC = PM10 - PM2_5
                                  ----------------------------------------------

                                  Note -
                                  This new compound is ONLY reported in the
                                  speciated tables below. In addition, output
                                  criteria emissions for the compound left of the
                                  subtraction operator are set to zero.
                                  ----------------------------------------------

     Species output list          :NO
                                  :NO2
                                  :OLE
                                  :PAR    …
                                  :FPRM
                                  :PEC
                                  :PNO3
                                  :POC

 Number of speciation factor records read:      513
 Number of unique speciation profiles stored:      103
 Number of pollutant conversion factor records read:      6
 Number of pollutant conversion factors stored:      6
 Number of speciation xref records read:      174
 Number of EMBR records processed:      4
 Number of records written to EMAR:       0
        ----------------------------------------------------------------
        Note:  Review the EPS3 Users Guide for a discussion of
               speciation issues.  In particular, a user must be
               aware of how input HCs have been reported (VOC,TOG,THC)
               and of air quality modeling requirements.  These input
               and output requirements determine which speciation and
               conversion factors should be used.
        ----------------------------------------------------------------
         Total Criteria Emissions Processed
                  English Tons

                      NOX         CO         VOC        PM10       PM2_5
        ----------------------------------------------------------------------
Input Emissions      585.8311    979.4699   1825.9321   5.0000     1.5000
 Output Criteria     585.8311    979.4699   1825.9321   0.         1.5000
 Output Speciated    585.8311    979.4698   1781.7369   0.         1.5000
 Emissions Skipped    0.          0.         0.         0.         0.
 Written to EMAR      0.          0.         0.         0.         0.
```

Exhibit 3-36. Example of a SPCEMS message file.

3.9 TMPRL

The TMPRL (**TeMP**o**R**a**L** allocation) module allows the user to introduce the degree of temporal resolution (i.e., hourly) required for the modeling inventory by the CAMx model. The primary functions of TMPRL are to

Adjust annual or seasonal average emissions to episodic levels,

Allocate emissions to the hours of the modeling episode, and

Generate an EMBR file containing hourly emissions data.

If the input EMBR file contains average daily emissions derived from annual data or average daily emissions for a specified period, these are first adjusted by applying a yearly profile to determine emissions levels for the episode month. The emissions are then adjusted for the day of week (Monday-Sunday) of the modeling episode based on weekly variations in activity levels. Finally, the episode-adjusted daily emissions are temporally allocated to each hour using a diurnal variation profile. Inventory types supported by TMPRL are:

AN	Annual	Month and day of week adjustments
PO	Peak ozone typical weekday	Adjustment for weekend days only
PC	Peak CO typical weekday	Adjustment for weekend days only
AD	Average day	Day of week adjustment only
S	Specified Interval	Adjustment depends on period interval

The SCC(ASC) code from each input emissions record is cross-referenced to a monthly, day of week, and diurnal profile code which determines the temporal profiles applied to the emissions. Although the default data supplied with the EPS3 distribution can be used with most applications, the user may want to update or refine this data to reflect activity patterns that are unique to the region of interest. To facilitate implementation of source- or geographical region-specific temporal profiles, the first three fields of each record in the cross-reference file allow the user to specify FIPS state and county codes, and AFS plant and stack identification codes for which the temporal profile should be applied, using the best match criteria described in Section 2.4. For each input EMBR record, TMPRL searches the cross-reference file to determine the assigned temporal profiles for the FIPS state/county codes, facility identification codes, and/or SCC(ASC) code combination most closely matching the input EMBR record. The user may define a global default temporal profile which will be applied to all EMBR records for which TMPRL cannot find a closer match using the following source identifying parameters:

FIPS state/county code:　　"00000" (all counties in modeling domain)
　　　　　　　　　　　　　　"*nn*000" (all counties in state *nn*)
Plant identification code:　　blank (all facilities in county)
Stack identification code:　　blank (all stacks in facility)
SCC(ASC):　　　　　　　　blank (all source categories)

Usually, the global default temporal profile will represent a flat activity profile (in other words, no monthly, weekly, or diurnal variations in activity levels). If an EMBR record contains an

⏎

SCC(ASC) code that cannot be cross-referenced to any temporal profile codes (including any specified global defaults), TMPRL writes the record to the output error file. These records can be inspected to determine what corrective actions may be taken.

> ➢ **Processing Tip**
> The TMPFAC utility should be run prior to executing TMPRL to ensure that any source-specific temporal data contained in the AFS file is incorporated into the temporal profiles and SCC(ASC)/ temporal profiles cross-reference files. This step is especially important to ensure that the operating schedule information contained on the AFS data record is utilized when processing point source inventory for temporal allocation. If the operating schedule information in the AFS file is unreliable or missing, the TMPFAC processing can be skipped and the TMPRL module will rely on default values to perform the temporal adjustments.

Input Files

The TMPRL module requires four input files. The first of these is the USERIN input file; TMPRL reads five packets from this file:

/TMPRL/ This packet (Table 3-26 and Exhibit 3-37) contains two parameters. The first parameter specifies the day of week for the modeling episode day ("MON", "TUE", "WED", "THU", "FRI", "SAT", or "SUN"). Recall that the EPS3 system does not support multi-day inventories. To produce emissions files for multiple days in the inventory the TMPRL module (and all succeeding modules) must be run for each day in the modeling episode. It is standard practice to produce a set of "representative" days for the modeling episode. Typically the representative days include a weekday, a Saturday and a Sunday for each season (Winter, Spring, Summer and Fall) of the modeling episode. The second parameter in the /TMPRL/ packet is the modeling time zone flag. This is used, together with the county time zone found in the /COUNTY/ packet, to adjust the hourly activity profiles to match the time zone used by the photochemical model. The CAMx model is always run within a single time zone. The activity data in any time zone different from the zone used by CAMx must be shifted to match the CAMx model. For example, suppose in a time zone one hour away from the time zone used by the CAMx model, a business begins operation at 9 AM. In the time zone used by the CAMx model it will only be 8 AM. The TMPRL module performs this shift by comparing the county specific time zone specified in the /COUNTY/ packet to the time zone specified in the /TMPRL/ packet. This flag can also be used to adjust for daylight savings time.

EPS3 will recognize US time zones (EST, EDT, CST, CDT, etc.) as well as global time zones. Global time zones are specified as an offset from Greenwich Mean Time (GMT). The convention used for specifiying global time zones is to use negative hourly offsets for the Western Hemisphere and positive offsets for the Eastern Hemisphere. For example, Eastern Standard Time (EST) could also be specified as GMT-5; Pacific Standard Time (PST) could be specified as GMT-8. Greenwich Mean Time is specified as GMT. Time zones which are offset from GMT by other than whole hours are not allowed.

Table 3-26. /TMPRL/ packet of EPS3 global user input file, USERIN.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	C	Packet identifier = /TMPRL/
2		1-20		Not used
	WEKDAY	21-30	C	Day of the week: MON, TUE, WED, THU, FRI, SAT, SUN
3		1-20		Not used
	INVTZ	21-30	C	Modeling Time Zone: PST, MST, CST, EST, PDT, MDT, CDT, EDT, GMT, GMT-5, etc.
4	KEYEND	1-20	C	Packet terminator = /END/

```
/TMPRL/
Day of Week        : MON
Time Zone          : CST
/END/
```

Exhibit 3-37. TMPRL packet of USERIN.

/DATE/   TMPRL reads the dates of the modeling episode from this packet (Table 2-6).

/COUNTY/ This packet is read to allow the module to check if a FIPS county code is valid for the modeling region. TMPRL also obtains the time zone of each county (Table 2-8). The module will perform a time shift for time zones different than that designated for the modeling domain.

/CRITERIA TABLES/ This packet (Table 2-11) specifies which criteria pollutant output tables, if any, the user wants to include in the output message file. See Section 2.4 for a full discussion on the output tables.

/SPECIES TABLES/ This packet (Table 2-11) specifies which chemical mechanism compound output tables, if any, the user wants to include in the output message file. See Section 2.4 for a full discussion on the output tables.

The second input file to TMPRL is the input EMBR file. This file can represent an inventory at any stage of the EPS processing; however, if an emissions record represents an hourly emissions total, TMPRL will write the record directly to the output file and resume execution at the next input record. That is, no adjustments are applied to hourly input data.

TMPRL also requires a file that cross-references SCC(ASC) codes to temporal profile codes (Table 3-27). The cross-reference file, which may be created with the TMPFAC utility, determines which temporal profiles will be applied to each source category. Each record contains source identification data (FIPS, facility identifiers, SCC/ASC) and AIRS pollutant code (SAROAD), followed by the monthly profile code, weekly profile code, and diurnal profile codes assigned to the source and pollutant (Exhibit 3-38). Although TMPRL supports the application of temporal profiles by pollutant code, it is typical practice to use the global code of all zeros to indicate that the profiles are to be used for all pollutants. For point sources, the temporal profiles may also use the facility, stack and point identifications for specific assignment of a profile based on the operating schedule.

Table 3-27. SCC(ASC)/temporal profiles cross-reference file (can be created by the TMPFAC utility).

Line	Variable	Columns	Type	Description
1+	FIPXRF	1-5	C	FIPS code of state/county: 00000 = applies to all counties in region *nn*000 = applies to all counties in state *nn* *nnmmm* = applies to county *mmm* in state *nn*
	SUBXRF	7-11	C	Subregion code (blank = applies to all subregions)
	FACXRF	13-17	C	AFS plant ID (blank = applies to all facilities in county)
	ISTXRF	19-21	C	AFS stack identification code (blank = applies to all stacks in facility)
	PNTID	23-25	C	Point identifier
	SCCXRF	27-36	C	Source Classification Code (SCC/ASC)
	INPOL	38-42	I	Pollutant code (00000 = all pollutants)
	IMNXRF	43-46	I	Monthly temporal profile code
	IWKXRF	47-50	I	Weekly temporal profile code
	IDYXRF	51-54	I	Diurnal temporal profile code

```
00000                                              00000 262   7  24
00000                                     10100101 00000 462   8  33
00000                                     10100102 00000 462   8  33
00000                                     10100201 00000 462   8  33
00000                                     10100202 00000 262   8  33
00000                                     10100203 00000 262   8  33
00000                                     10100204 00000 262   8  33
00000                                     10100205 00000 462   8  33
00000                                     10100211 00000 262   8  33
00000                                     10100212 00000 266   8  33
00000                                     10100215 00000 262   8  33
00000                                     10100217 00000 462   8  33
00000                                     10100218 00000 262   8  33
00000                                     10100221 00000 262   8  33
00000                                     10100222 00000  34   8  33
00000                                     10100223 00000 262   8  33
```

Exhibit 3-38. Example of temporal allocation cross reference file input to TMPRL.

The fourth input file, which can also be created with the TMPFAC utility, contains the temporal profiles data used to adjust the data to episodic levels and allocate daily emissions to the hours of the modeling episode (Exhibit 3-39). TMPRL accesses these profiles using the temporal profile code, the first field on each record. Similar to the USERIN, the temporal profiles file is split into packets: /MONTHLY/, /WEEKLY/, /DIURNAL WEEKDAY/, and /DIURNAL WEEKEND/ (Tables 3-28 through 3-30). Note that although separate packets are provided for weekday and weekend diurnal allocation profiles, only one diurnal profile code is specified in the SCC(ASC)/temporal profiles cross-reference file. If the user specifies "SAT" or "SUN" as the episode day in the /TMPRL/ packet of USERIN, and the assigned diurnal profile code for that source is not included in the /DIURNAL WEEKEND/ packet, TMPRL will default to the corresponding profile in the /DIURNAL WEEKDAY/ packet. Data need be included in the /DIURNAL WEEKEND/ packet for only those profiles in which the activity varies from a weekday to a weekend day.

The temporal profile data contained in all four packets are represented in the same manner; each time interval (month, day of week, or hour) of the profile contains a weight factor that indicates the level of operation throughput or activity with respect to the other time intervals in the profile. The last field contains the total weight for all time intervals in the period type (i.e. all months of the year). TMPRL will calculate a factor for each time interval by dividing the weight for the time interval by the total weight for all time intervals. This method allows the monthly weights to be applied correctly to a seasonal inventory.

> ➢ **Temporal Adjustment Example**
> The monthly temporal adjustment factor for an August episode would be calculated by dividing the weight factor for August by the total weight factor for all 12 months. The result, representing the fraction of annual activity occurring in August, is multiplied by the number of comparable time periods for which the data was compiled (12 if the data represents annual average emissions, 3 if it represents average emissions for a 3-month ozone season, etc.) to obtain the final monthly adjustment factor. This means that if the weight for August is more than 1/12 (for an annual average inventory) of the total weight, the emission rate will actually be increased.

```
/MONTHLY/
    1  83   83   83   83   83   83   83   83   83   83   83   996
    2  79   79   82   83   84   84   85   87   85   84   84   84 1000
    6 190  238  238  190    0    0    0    0    0    0   24  119  999
    8  61   73   98  122   98   73   61   61   73  122   98   61 1001
   13   0    0   15   74  147  147  147  147  147  147   29    0 1000
   14   0    0  167  333  333    0    0    0    0    0    0  167 1000
   22 250  250  250    0    0    0    0    0    0   83   83   83  999
   30  67   67   83   83   83  100  100  100   83   83   83   67 1200
  213  67   67   83   83   83   92   92   92   92   92   92   67 1104  coil coating
/END/

/WEEKLY/
    1   1   1   1   1   1   0   0    5
    5   1   1   1   1   1   0   0    5
    4   1   1   1   1   1   0   0    5
  209  18  18  18  18  18   9   0   99  auto repair
  210  19  19  19  19  19   2   0   97  auto refinishing
  212  16  16  16  16  16   8   8   96  can coating
/END/

/DIURNAL WEEKDAY/
    6   0   0   0   0   0   0   1   1   1   1   1   1   0   0   0   0   0   0   0   0   0   0   0   0    6
    7   0   0   0   0   0   0   0   0   0   1   1   1   1   1   1   1   0   0   0   0   0   0   0   0    7
   26 198 186 182 187 210 250 311 388 467 528 571 604 620 631 635 624 594 548 531 509 425 327 257 21810001
   27  23  23  23  23  23  23  15  15  15  15  15  15  15  15  15  15  15  15  15  15  15  15  23  23  424
   31   3   1   1   1   1   1   1   5   5   5   5   5   5   5   5   5   5  10  10  10  10   7   7   3  116
   33   2   2   2   2   2   2   2  10  10   6   6   5   5   5   5   5   5   5  10  10  10  10   2  128
   34   0   8   8   8   8  10  10  10  10   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   72
   60  17  17  17  17  17  17  48  48  48  48  48  48  48  48  48  48  48  48  48  48  48  48  48  48  966
  215   0   0   0   0   0   0   0  20  82  82 102 102 102 102 102 102 102  82  20   0   0   0   0   0 1000
  218  30  30  30  30  30  30  61  61  61  61  61  61  61  61  61  30  30  30  30  30  30  30  30  30  999
/END/

/DIURNAL WEEKEND/
   50   9   1   1   1   1   7   9  32  43  51  97  84  89  80  78  77  89  72  44  42  41  20  20   8  996
  202   0   0   0   0   0   0   1   1   1   1   1   1   1   1   1   1   1   0   0   0   0   0   0   0   12
  203   0   0   0   0   0   0   0   0   1   1   1   1   1   1   1   1   1   0   0   0   0   0   0   0    9
  205   0   0   0   0   0   0   0   0  67 133 133 133  67  67  67  67  67  67  67  67   0   0   0   0 1000
  217  30  30  30  30  30  30  30  30  61  61  61  61  61  61  61  61  61  30  30  30  30  30  30  30 1000
/END/
```

Exhibit 3-39. Example of temporal profiles file input to TMPRL.

Table 3-28. /MONTHLY/ packet of temporal factors file (can be created by the TMPFAC utility) read by the TMPRL module.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	C	Packet identifier = /MONTHLY/
2+	IMNCD	1-5	I	Monthly temporal profile code
	IMNFAC(1)	6-9	I	Temporal weight for month of January
	IMNFAC(2)	10-13	I	Temporal weight for month of February
	.			
	.			
	.			
	IMNFAC(12)	50-53	I	Temporal weight for month of December
	IMNTOT	54-58	I	Total of weights for entire year
3	KEYEND	1-20	C	Packet terminator = /END/

Table 3-29. /WEEKLY/ packet of temporal factors file (can be created by the TMPFAC utility) read by the TMPRL module.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	C	Packet identifier = /WEEKLY/
2+	IWKCD	1-5	I	Weekly temporal profile code
	IWKFAC(1)	6-9	I	Temporal weight for Monday
	IWKFAC(2)	10-13	I	Temporal weight for Tuesday
	.			
	.			
	.			
	IWKFAC(7)	30-33	I	Temporal weight for Sunday
	IWKTOT	34-38	I	Total of weights for entire week
3	KEYEND	1-20	C	Packet terminator = /END/

Table 3-30. /DIURNAL WEEKDAY/ and /DIURNAL WEEKEND/ packets of temporal factors file (can be created by the TMPFAC utility) read by the TMPRL module.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	C	Packet identifier - /DIURNAL WEEKDAY/, or /DIURNAL WEEKEND/
2+	IDYCD	1-5	I	Diurnal temporal profile code
	IDYFAC(1)	6-9	I	Temporal weight for hour beginning 0000
	IDYFAC(2)	10-13	I	Temporal weight for hour beginning 0100
	.			
	.			
	.			
	IDYFAC(24)	98-101	I	Temporal weight for hour beginning 2300
	IMNTOT	102-106	I	Total of weights for entire day
3	KEYEND	1-20	C	Packet terminator - /END/

Output Files

TMPRL produces three output files: a message file, an EMBR file, and an EMAR error file. The first section of the message file consists of a summary of input and output file names, episode definition parameters, selected user options (standard or daylight savings time, day of week, etc.), and number of profiles for each profile type; this section may also include warning messages. Following this section is a summary of domain-wide input and output criteria pollutant emissions totals. The final section of the message output file contains tabular output as indicated in the

indicated in the USERIN /CRITERIA TABLES/ and /SPECIES TABLES/ packets. Exhibit 3-40 shows an example of the TMPRL message file.

The EMBR output file produced by TMPRL contains hourly emissions for each source; this file contains many more records than the EMBR input file. To save space, the TMPRL module will not create a record in the EMBR file for each hour. Instead, it will create a record for an entire period for which the emission rate is constant. Because the hourly profiles are typically step functions, there are usually sections of the day (sometimes the entire day) when the emission rate is constant. TMPRL will write a single record for this period with an emission rate representing the entire period.

The third output file, in EMAR format, contains records that could not be processed. The user should examine the records in this file to determine the action needed to rectify any processing problems.

Exhibit 3-41 shows an example of a TMPRL job script.

```
                    EPS3 TMPRL module v. 1.01 Oct 2004       07/25/07 18:41:52

            Input Files
     USERIN file                     :../inputs/userin.test_problem.wkd
     Input EMBR file                 :../embr/embr.chmspl.ar.test_problem
     ASC-SCC/temporal code xref fil:../inputs/temporal.allocation.xref_area.Aug03
     Temporal profiles file          :../inputs/temporal.profiles.Aug03


            Output Files
     Output EMBR file                :../embr/embr.tmprl.ar.test_problem.wkd
     EMAR error file                 :../error/emar.tmprl.ar.test_problem.wkd


                    EPS3 TMPRL module v. 1.01 Oct 2004       07/25/07 18:41:52

     File note                       :CAMx Modeling of Tx regional, 9/13/99
     Episode date (Calander)         :990913
     Episode date (Julian)           :99256
     Beginning hour                  :     0
     Ending hour                     :    24
     Number of counties              :   213
     Day of week                     :MON
     Inventory Timezone :            :CST


     Number of ASC-SCC/temporal profile cross reference records read:   509
     Number of ASC-SCC/temporal profile cross reference entries:   499
     Number of MONTHLY temporal profiles read:     26
     Number of WEEKLY temporal profiles read:     20
     Number of DIURNAL WEEKDAY temporal profiles read:    70
     Number of DIURNAL WEEKEND temporal profiles read:    11
     Number of input records read:    12293
     Number of input records written to EMAR:         0
     Number of skipped records:        0
     Number of output records written:    45577

                 Total Emissions Processed
                      English Tons


                           NOX          CO          VOC
          -------------------------------------------------------
     Input Emissions        585.8311    979.4699    1825.9321
     Output Emissions       585.8311    979.4699    1825.9227
     Written to EMAR          0.          0.          0.
     Emissions Skipped        0.          0.          0.
          -------------------------------------------------------

                   Criteria Pollutant Emissions by Hour
                          English Tons/Hour


     Hour      Input       Output      Input       Output      Input       Output
               NOX         NOX         CO          CO          VOC         VOC
          --------------------------------------------------------------------------
      01      24.4096     22.3460     40.8112     22.7487     76.0800     38.3126
      02      24.4096     22.3460     40.8112     22.7487     76.0800     38.3126
      03      24.4096     22.3460     40.8112     22.7487     76.0800     38.3126
      04      24.4096     22.3460     40.8112     22.7487     76.0800     38.3126
      05      24.4096     22.3460     40.8112     22.7487     76.0800     38.3126
      06      24.4096     22.3460     40.8112     22.7487     76.0800     39.0064
      07      24.4096     23.1060     40.8112     47.8286     76.0800     64.2986
      08      24.4096     25.3111     40.8112     49.4671     76.0800     99.5482
      09      24.4096     25.8614     40.8112     57.9064     76.0800    111.8728
      10      24.4096     25.5920     40.8112     57.3013     76.0800    108.5338
```

Exhibit 3-40. Example of a TMPRL message file.

```
#!/bin/csh
#
#    --- Sample job script for running the
#        EPS3 module TMPRL
#
set EXEC = /models/eps3/src
#
set SCENARIO = test_problem
#
foreach DAY (wkd sat sun)
#
rm -f ../msg/msg.tmprl.ar.$SCENARIO.$DAY
rm -f ../embr/embr.tmprl.ar.$SCENARIO.$DAY
rm -f ../error/emar.tmprl.ar.$SCENARIO.$DAY
#
echo "--------------------------------------------------"
echo "    Running TMPRL for $SCENARIO - area sources"
echo "          Day - $DAY"
echo "--------------------------------------------------"
#
$EXEC/tmprl/tmprl << IEOF
USERIN file        :../inputs/userin.$SCENARIO.$DAY
Input EMBR file    :../embr/embr.chmspl.ar.$SCENARIO
ASC-SSC/tmprl XRF  :../inputs/temporal.allocation.xref_area.Aug03
Temporal profiles  :../inputs/temporal.profiles.Aug03
Output Messages    :../msg/msg.tmprl.ar.$SCENARIO.$DAY
Output SCC/stacks  :../embr/embr.tmprl.ar.$SCENARIO.$DAY
EMAR error file    :../error/emar.tmprl.ar.$SCENARIO.$DAY
IEOF
end
```

Exhibit 3-41. Example of a TMPRL job script.

3.10 PSTFIR

The EPS3 PSTFIR (**PoST** processor for **FIR**e source emissions) module is required to generate the output fire emissions loaded by PREFIR. The primary functions of PSTFIR are

Determine fraction of fire emissions in surface layer,

Assign surface fire emissions to grid cells based on fire source location,

Determine plume characteristics of source based on fire size,

Distribute non-surface emissions through vertical layers,

Create a CAMx model-ready surface emissions file,

Create an ASCII 'stack' list of elevated fire point sources,

Create an ASCII fire emissions file of elevated fire sources, and

To provide the user with tabular summaries of fire source emissions to assist in quality control tracking.

PSTFIR reads the speciated, temporally allocated EMBR file and generates output files for both the surface layer and the elevated source files. Only those EMBR records with a record type "F" (for "fire") are processed. In addition, only records with a state/county code specified in the /COUNTY/ packet of the USERIN are processed. PSTFIR will write a warning message to the message output file if no EMBR records are found for a county listed in the /COUNTY/ packet.

PSTFIR is executed after all other processing of the fire source data, prior to PIGEMS and MRGUAM. It determines and outputs surface fire emissions as well as elevated location specific, with vertical resolution, fire emissions.

Fire Class and Plume Characteristics

Each EMBR record has a fire class, based on fire virtual acreage, assigned when the fire source emissions are loaded by PREFIR. The fire class is stored on the EMBR record in the 'stack diameter' field. The algorithms and factors that are incorporated in the PSTFIR module are taken from the WRAP 2002 Phase II EI Report dated 22 July 2005. Table 3-31 indicates buoyant efficiency as a function of hour and is provided for reference. These values are inherent to the fire source calculations and are not user defined.

Table 3-31. Buoyant Efficiency as a Function of Hour.

Hour	1	2	3	4	5	6	7	8	9	10	11	12
BE	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.06	0.10	0.2	0.4
Hour	13	14	15	16	17	18	19	20	21	22	23	24
BE	0.7	0.8	0.9	0.95	0.99	0.8	0.7	0.4	0.06	0.03	0.03	0.03

The fire class size determines the fraction of the fire emissions put in the surface layer. Surface emissions are calculated every hour and determined with:

$$\text{Surface}_{hour} = 1 - (BE_{hour} * BE_{size})$$

Where BE represents the buoyant efficiency by hour (Table 3-31) and fire size (defaults in Table 3-7).

The non-surface emissions are distributed vertically based on the hourly top and bottom plume heights. The heights are calculated with:

$$\text{PlumeTop}_{hour} = (BE_{hour})^2 * (BE_{size})^2 * Ptop_{size}$$
$$\text{PlumeBot}_{hour} = (BE_{hour})^2 * (BE_{size})^2 * Pbot_{size}$$

Where BE is defined as above and Ptop and Pbot are the plume top and bottom based on fire size (defaults in Table 3-7). The hourly emissions are distributed to the vertical layers on a weighted average based on layer thickness. The vertical layer structure is specified in the /LAYERS/ packet of the USERIN.

Input Files

PSTFIR requires two input files: USERIN and an EMBR fire source emissions file. PSTFIR reads the following packets from USERIN:

/LAYERS/   This packet (Table 3-32) provides the vertical layer structure for generating the layer specific elevated fire source emissions. The layers must be specified in increasing heights where the specified height indicates the top of the layer above ground level. (Exhibit 3-42)

Table 3-32. /LAYERS/ packet of EPS3 global user input file, USERIN.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	C	Packet identifier - /LAYERS/
2+		1-20		Not used
	AGLHT()	21-30	R	Height above ground level (m)
3	KEYEND	1-20	A	Packet terminator - /END/

```
/LAYERS/
Ht AGL (m) Layer 1 : 39.
Ht AGL (m) Layer 2 : 79.
Ht AGL (m) Layer 3 : 119.
Ht AGL (m) Layer 4 : 159.
Ht AGL (m) Layer 5 : 239.
Ht AGL (m) Layer 6 : 321.
Ht AGL (m) Layer 7 : 403.
Ht AGL (m) Layer 8 : 485.
Ht AGL (m) Layer 9 : 652.
Ht AGL (m) Layer 10: 822.
Ht AGL (m) Layer 11: 994.
Ht AGL (m) Layer 12: 1170.
Ht AGL (m) Layer 13: 1530.
Ht AGL (m) Layer 14: 1998.
Ht AGL (m) Layer 15: 2692.
Ht AGL (m) Layer 16: 3775.
Ht AGL (m) Layer 17: 5661.
Ht AGL (m) Layer 18: 8950.
Ht AGL (m) Layer 19: 16350.
/END/
```

Exhibit 3-42. Example of a /LAYERS/ packet of USERIN file.

/FIRE BINS/ PSTFIR reads the /FIRE BINS/ packet whose format is specified in the PREFIR Section 3.4 (Table 3-9). If the packet is not provided then the defaults specified in Table 3-7 will be used. This packet allows the user to specify non-default fire class sizes and parameters. Since the fire class is determined and set at the PREFIR stage it is imperative that this packet NOT be modified after PREFIR is run. Exhibit 3-13 is an example of the /FIRE BINS/ packet specifying the default parameters.

/SPECIES LIST/ This packet (Table 2-11) provides the species list for air quality modeling.

/DATE/ This packet (Table 2-6) provides the modeling episode information.

/REGION/ PSTFIR uses this packet's data (Table 2-7) to determine if any points in the input EMBR file lie outside of the modeling domain. If such sources are encountered, they will be skipped.

/COUNTY/ PSTFIR reads this packet (Table 2-8) to check the county identification code specified on each input record against the region county list, and to determine if any counties from the region list had no corresponding EMBR data records.

/CRITERIA TABLES/ This packet (Table 2-11) specifies which criteria pollutant output tables, if any, the user wants to include in the output message file. See Section 2.4 for a full discussion on the output tables.

/SPECIES TABLES/ This packet (Table 2-11) specifies which chemical mechanism compound

output tables, if any, the user wants to include in the output message file. See Section 2.4 for a full discussion on the output tables.

The second input file to PSTFIR is the EMBR file containing location specific fire source emissions data. The data in this file must be temporally allocated by hour (by the TMPRL module) and chemically speciated (SPCEMS or CHMSPL).

Output Files

PSTFIR creates five output files; a summary message file, two optional elevated emissions files (the list of 'stacks' and corresponding elevated emissions which are required by the PIGEMS module), a surface CAMx emissions file, and an EMAR formatted errors file.

The PSTFIR message file summarizes fire source emissions (Exhibit 3-44). The first section of the message file summarizes input and output file names, region definition parameters, the beginning and ending dates and times for the emissions data contained in the output file, fire bin parameters, and the output emissions species list. The next section lists domain-wide totals of criteria pollutants and chemical mechanism compounds for both input and output emissions (including both surface and elevated sources). This is followed by a table of output criteria emissions by fire class, and another table by vertical layer. These may be followed by a series of warning messages indicating counties specified in the /COUNTY/ packet of USERIN for which no records were found in the input EMBR file. The final section provides emissions totals tables as specified in the USERIN packets, /CRITERIA TABLES/ and /SPECIES TABLES/.

If the job script specifies file names for the output elevated emissions and stack header files then these files will be created. If the file names are blank then no output elevated sources will be written. This allows the user to run PSTFIR multiple times; once to generate regional domain elevated sources and a surface file, and additional times to just generate the surface file for a smaller region definition.

The output stack list file contains the information needed to uniquely identify each fire source, including FIPS, 'facility' and 'stack' identification codes, coordinates, and stack parameter information including stack height, exit temperature, diameter, exit velocity and flowrate (Exhibit 3-45). This file format is identical to PSTPNT outputs which are detailed in the next module section. Fire emissions have no real 'stack' parameters. Instead PSTFIR calculates the plume as outlined above and generates unique output records, one for each vertical layer with non-zero emissions. The mid-point of the vertical layer is indicated as a negative (-) stack height which informs PIGEMS never to P-I-G the source. The other stack parameters are all set to 1.0.

The stack emissions file, similar in format to PSTPNT output shown in Exhibit 3-52 contains the stack identifiers, stack parameters, coordinates,episode date, parent criteria pollutant name, air quality modeling compound name, and 24-hourly emission rates for each elevated fire source.

The CAMx surface emissions file, always generated by PSTFIR, contains the computed surface fire emissions for the modeling region specified in the /REGION/ packet. This file can be input to MRGUAM. Similar to GRDEM, PSTFIR should be run multiple times, one for each grid resolution in order to incorporate the surface fire emissions in each grid.

The final output file is the EMAR error file that contains records that could not be processed.

Exhibit 3-43 shows an example of a PSTFIR job script.

```
#!/bin/csh
#
#   --- Sample job script for running the
#       EPS3 module PSTFIR
#
set EXEC = /models/eps3/src
#
set SCENARIO = 2005_07_02
#
rm -f ../emiss/camx.surface.fire_pts.$SCENARIO
rm -f ../emiss/elvems.fire_pts.$SCENARIO
rm -f ../emiss/stkhdr.fire_pts.$SCENARIO
rm -f ../error/emar.pstfir.fire_pts.$SCENARIO
rm -f ../msg/msg.pstfir.fire_pts.$SCENARIO
#
echo "--------------------------------------------------"
echo "     Running PSTFIR for $SCENARIO - point sources"
echo "--------------------------------------------------"

$EXEC/pstfir/pstfir << IEOF
USERIN file        :../inputs/userin.$SCENARIO
Input EMBR file    :../embr/embr.tmprl.pts.$SCENARIO
Output Messages    :../msg/msg.pstfir.fire_pts.$SCENARIO
Output ELEV Emiss  :../emiss/elvems.fire_pts.$SCENARIO
Output Stack/HDR   :../emiss/stkhdr.fire_pts.$SCENARIO
Output Surface CAMx:../emiss/camx.surface.fire_pts.$SCENARIO
EMAR error file    :../error/emar.pstfir.fire_pts.$SCENARIO
IEOF
end
```

Exhibit 3-43. Example of a PSTFIR job script.

```
              EPS3 PSTFIR module v. 1.00 Jun 2008

          Input Files
     USERIN file                      :../../inputs/userin.2005_07_06
     Input EMBR file                  :embr.tmprl.2005_07_06

          Output Files
     Message file                     :msg.pstfir.2005_07_06
     Elevated emissions file          :elv.pstfir.2005_07_06
     Elevated header file             :hdr.pstfir.2005_07_06
     Surface emissions file           :srf.pstfir.2005_07_06
     ERROR file                       :emar.pstfir.2005_07_06

              EPS3 PSTFIR module v. 1.00 Jun 2008      08/18/08 13:30:49


     File note                        :CAMx Fires Test Case
     Episode date (Calander)          : 50605
     Episode date (Julian)            : 5156
     Beginning hour                   :    0
     Ending hour                      :   24
     Grid origin (km)                 : (  -108.000,  -1584.000)
     UTM zone                         :    0
     Grid cell width (km)             : (    36.000,     36.000)
     Number of cells                  : (  69,   67)
     Number of counties               :   96
     Specified Fire Bins              : None - Defaults Assigned
                                        Class    Size      BE   PtopMax   PbotMax
                                          1      10.0    0.400    160.0      0.0
                                          2     100.0    0.600   2400.0    900.0
                                          3    1000.0    0.750   6400.0   2200.0
                                          4    5000.0    0.850   7200.0   3000.0
                                          5    9999.0    0.900   8000.0   3000.0


     Layer AGL Ht (m)                 :       39.62 ( 1)
                                      :       79.38 ( 2)
                                      :      119.30 ( 3)
                                      :       etc

     Species output list             :NO
                                      :NO2
                                      :OLE
                                      :PAR
                                      :TOL
                                      :XYL
                                      :FORM
                                      :  etc

          Total Emissions Processed
               English Tons

                        NOX          CO          VOC
     -----------------------------------------------------------
     Input Emissions     2405.7701  1071.6300     646.8701
     Output Emissions    2084.9501   854.0600     172.2500
     Low Level Emissions  320.8200   217.5700     474.6200
     Written to EMAR          0.          0.          0.
     Emissions Skipped    320.8200   217.5700     474.6200
     -----------------------------------------------------------
```

Exhibit 3-44. Example of a PSTFIR message file.

```
ORIGINAL    01000    F00000001  SL001          -19.8    1.000       1.        1.    1022000.    -554000.
ORIGINAL    01000    F00000001  SL002          -59.5    1.000       1.        1.    1022000.    -554000.
ORIGINAL    01000    F00000001  SL003          -99.3    1.000       1.        1.    1022000.    -554000.
ORIGINAL    01000    F00000001  SL004         -139.3    1.000       1.        1.    1022000.    -554000.
ORIGINAL    01000    F00000001  SL005         -199.7    1.000       1.        1.    1022000.    -554000.
ORIGINAL    01000    F00000001  SL006         -280.6    1.000       1.        1.    1022000.    -554000.
ORIGINAL    01000    F00000001  SL007         -362.1    1.000       1.        1.    1022000.    -554000.
ORIGINAL    01000    F00000001  SL008         -444.3    1.000       1.        1.    1022000.    -554000.
ORIGINAL    01000    F00000001  SL009         -569.0    1.000       1.        1.    1022000.    -554000.
ORIGINAL    01000    F00000001  SL010         -737.3    1.000       1.        1.    1022000.    -554000.
ORIGINAL    01000    F00000001  SL011         -908.4    1.000       1.        1.    1022000.    -554000.
ORIGINAL    01000    F00000001  SL012        -1082.4    1.000       1.        1.    1022000.    -554000.
ORIGINAL    01000    F00000001  SL013        -1350.1    1.000       1.        1.    1022000.    -554000.
ORIGINAL    01000    F00000001  SL014        -1764.3    1.000       1.        1.    1022000.    -554000.
ORIGINAL    01000    F00000001  SL015        -2345.7    1.000       1.        1.    1022000.    -554000.
ORIGINAL    01000    F00000001  SL016        -3234.2    1.000       1.        1.    1022000.    -554000.
ORIGINAL    01000    F00000002  SL001          -19.8    1.000       1.        1.     874000.    -710000.
ORIGINAL    01000    F00000002  SL002          -59.5    1.000       1.        1.     874000.    -710000.
ORIGINAL    01000    F00000002  SL003          -99.3    1.000       1.        1.     874000.    -710000.
ORIGINAL    01000    F00000002  SL004         -139.3    1.000       1.        1.     874000.    -710000.
ORIGINAL    01000    F00000002  SL005         -199.7    1.000       1.        1.     874000.    -710000.
ORIGINAL    01000    F00000002  SL006         -280.6    1.000       1.        1.     874000.    -710000.
ORIGINAL    01000    F00000002  SL007         -362.1    1.000       1.        1.     874000.    -710000.
ORIGINAL    01000    F00000002  SL008         -444.3    1.000       1.        1.     874000.    -710000.
ORIGINAL    01000    F00000002  SL009         -569.0    1.000       1.        1.     874000.    -710000.
ORIGINAL    01000    F00000002  SL010         -737.3    1.000       1.        1.     874000.    -710000.
ORIGINAL    01000    F00000002  SL011         -908.4    1.000       1.        1.     874000.    -710000.
ORIGINAL    05000    F00000003  SL001          -19.8    1.000       1.        1.     498000.    -734000.
ORIGINAL    05000    F00000003  SL002          -59.5    1.000       1.        1.     498000.    -734000
```

Exhibit 3-45. Example of stack header file created by PSTFIR and input to PIGEMS.

3.11 PSTSHP

The EPS3 PSTSHP (**P**o**ST** processor for **SH**i**PP**ing source emissions) module is required to generate the output shipping emissions loaded by PRESHP. The primary functions of PSTSHP are

    Distribute emissions through vertical layers,

    Create a CAMx model-ready surface emissions file,

    Create an ASCII 'stack' list of elevated shipping sources, and

    Create an ASCII shipping emissions file of elevated shipping sources.

PSTSHP reads the speciated, temporally allocated EMBR file and generates output files for both the surface layer and the elevated source files. Only those EMBR records with a record type "S" (for "shipping") are processed. In addition, only records with a state/county code specified in the /COUNTY/ packet of the USERIN are processed. PSTSHP will write a warning message to the message output file if no EMBR records are found for a county listed in the /COUNTY/ packet.

The PSTSHP module determines the distribution of shipping emissions to vertical layers. Emissions distributed to the lowest layer will be written to the CAMx surface emissions file. All other shipping emissions are written to the elevated files, the stack list and corresponding elevated emission file.

PSTSHP is executed after all other processing of the shipping source data, prior to PIGEMS and MRGUAM. It determines and outputs surface shipping emissions as well as elevated location specific, with vertical resolution, shipping emissions.

> ➢ **Note**
> Instead of running PSTSHP which will generate both surface and elevated emissions files, a user has the option of running GRDEM to generate a surface emissions file that contains all shipping emissions.

Input Files

PSTSHP requires three input files: USERIN, an EMBR shipping source emissions file, and the vessel/stack cross reference file. PSTSHP reads the following packets from USERIN:

/LAYERS/   This packet (also used in PSTFIR, Table 3-32) provides the vertical layer structure for generating the layer specific elevated shipping source emissions. The layers must be specified in increasing heights where the specified height indicates the top of the layer above ground level. (Exhibit 3-42)

/SPECIES LIST/ This packet (Table 2-11) provides the species list for air quality modeling.

/DATE/   This packet (Table 2-6) provides the modeling episode information.

/REGION/   PSTSHP uses this packet's data (Table 2-7) to determine if any points in the input
              EMBR file lie outside of the modeling domain. If such sources are encountered,
              they will be skipped.

/COUNTY/   PSTSHP reads this packet (Table 2-8) to check the county identification code
              specified on each input record against the region county list, and to determine if
              any counties from the region list had no corresponding EMBR data records.

/CRITERIA TABLES/ This packet (Table 2-11) specifies which criteria pollutant output tables,
              if any, the user wants to include in the output message file. See Section 2.4 for a full
              discussion on the output tables.

/SPECIES TABLES/ This packet (Table 2-11) specifies which chemical mechanism compound
              output tables, if any, the user wants to include in the output message file. See
              Section 2.4 for a full discussion on the output tables.

The second input file to PSTSHP is the EMBR file containing gridded (via PRESHP), hourly
shipping emissions data. The data in this file must be temporally allocated by hour (by the
TMPRL module) and chemically speciated (SPCEMS or CHMSPL).

The third input file, SCC/vessel cross reference, specifies the bottom and top plume heights by
SCC and vessel type. This file is essentially a lookup table that assigns an appropriate plume to
each source category code and vessel type. Plume heights for ship emissions are specified as a
physical height in meters (e.g., 100 m) which PSTSHP converts to CAMx layer using user input
data (/LAYERS/ packet) for the layer heights.   The best match hierarchy is supported. Table 3-
33 and Exhibit 3-46 indicate the file format and an example file respectively.

Table 3-33. SCC/vessel type cross-reference file.

Line	Variable	Columns	Type	Description
1+	ASCMAP	1-10	C	Source Classification Code (SCC)
	VSLMAP	12-21	C	Vessel type code (optional).
	PLUMEBOT	23-32	R	Bottom of the plume height estimate (m).
	PLUMETOP	34-43	R	Top of the plume height estimate (m).

```
2280000000                34.0        58.0
2280001000                34.0        58.0
2280001010                40.0        60.0
2280001010    LCruise     50.0        60.0
2280001010    Tanker      55.0        60.0
2280001020    Tug          8.0        10.0
2280001040    CARRIER     40.0        55.0
2280002000                34.0        58.0
2280002010                40.0        60.0
2280001010    LCruise     50.0        60.0
2280001010    Tanker      55.0        60.0
2280002020                 4.0        10.0
2280001020    Tug          8.0        10.0
```

Exhibit 3-46. Example of SCC/vessel cross reference file read by PSTSHP.

Output Files

PSTSHP creates five output files; a summary message file, two elevated emissions files (the list of 'stacks' and corresponding elevated emissions which are required by the PIGEMS module), a surface CAMx emissions file, and an EMAR formatted errors file.

The PSTSHP message file summarizes the shipping source emissions (Exhibit 3-48). The first section of the message file summarizes input and output file names, region definition parameters, the beginning and ending dates and times for the emissions data contained in the output file, the user specified vertical layer structure, and the output emissions species list. The next section lists domain-wide totals of criteria pollutants and chemical mechanism compounds for both input and output emissions (including both surface and elevated sources). This is followed by a table of output criteria emissions by vertical layer. These may be followed by a series of warning messages indicating counties specified in the /COUNTY/ packet of USERIN for which no records were found in the input EMBR file. The final section provides emissions totals tables as specified in the USERIN packets, /CRITERIA TABLES/ and /SPECIES TABLES/. There is one additional table that is included, a table of emissions by SCC and vertical layer. This table will be written if, and only if, the user requests the SCC output table.

The output stack list file contains the information needed to uniquely identify each shipping source, including FIPS, 'facility' and 'stack' identification codes, coordinates, and stack parameter information including stack height, exit temperature, diameter, exit velocity and flowrate (Exhibit 3-51). This file format is identical to PSTPNT outputs which are detailed in the next module section. Shipping emissions have no real 'stack' parameters. Instead PSTSHP determines the plume as outlined above and generates unique output records, one for each vertical layer with non-zero emissions. The mid-point of the vertical layer is indicated as a negative (-) stack height which informs PIGEMS never to P-I-G the source. The other stack parameters are all set to 1.0.

The stack emissions file, similar in format to PSTPNT output shown in Exhibit 3-52 contains the stack identifiers, stack parameters, coordinates,episode date, parent criteria pollutant name, air quality modeling compound name, and 24-hourly emission rates for each elevated shipping source.

The CAMx surface emissions file contains the computed surface fire emissions for the modeling region specified in the /REGION/ packet. This file can be input to MRGUAM. Similar to GRDEM, PSTSHP should be run multiple times, one for each grid resolution in order to incorporate the surface shipping emissions in each grid.

> ➢ **Note**
> When running PSTSHP multiple times, once for each modeling grid, only the largest regional domain **elevated** point source files should be used in the PIGEMS point source merging module. If all elevated files were merged, one for each nested grid, the emissions would be double counted in the overlaying grid areas.

The final output file is the EMAR error file that contains records that could not be processed.

Exhibit 3-47 shows an example of a PSTSHP job script.

```
#!/bin/csh
#
#    --- Sample job script for running the
#        EPS3 module PSTSHP
#
set EXEC = /models/eps3/src
#
set SCENARIO = 2005_07_02
#
rm -f ../emiss/camx.surface.ship.$SCENARIO
rm -f ../emiss/elvems.ship.$SCENARIO
rm -f ../emiss/stkhdr.ship.$SCENARIO
rm -f ../error/emar.pstshp.ship.$SCENARIO
rm -f ../msg/msg.pstshp.fire_pts.$SCENARIO
#
echo "-------------------------------------------------"
echo "  Running PSTSHP for $SCENARIO - shipping sources"
echo "-------------------------------------------------"

$EXEC/pstshp/pstshp << IEOF
USERIN file        :../inputs/userin.$SCENARIO
Input EMBR file    :../embr/embr.tmprl.ship.$SCENARIO
Vessel/Stack XREF  :../inputs/vessel_stack.xrf
Output Messages    :../msg/msg.pstfir.ship.$SCENARIO
Output ELEV Emiss  :../emiss/elvems.ship.$SCENARIO
Output Stack/HDR   :../emiss/stkhdr.ship.$SCENARIO
Output Surface CAMx:../emiss/camx.surface.ship.$SCENARIO
EMAR error file    :../error/emar.pstshp.ship.$SCENARIO
IEOF
end
```

Exhibit 3-47. Example of a PSTSHP job script.

```
                EPS3 PSTSHP module v. 3.11 Jun 2009


          Input Files
    USERIN file                      :../../inputs/userin.2005_07_06
    Input EMBR file                  :embr.tmprl.2005_07_06

          Output Files
    Message file                     :msg.pstship.2005_07_06
    Elevated emissions file          :elv.pstshp.2005_07_06
    Elevated header file             :hdr.pstshp.2005_07_06
    Surface emissions file           :srf.pstshp.2005_07_06
    ERROR file                       :emar.pstshp.2005_07_06

              EPS3 PSTFIR module v. 3.11 Jun 2009      07/18/09 13:30:49


    File note                        :CAMx Shipping Test Case
    Episode date (Calander)          : 50605
    Episode date (Julian)            : 5156
    Beginning hour                   :     0
    Ending hour                      :    24
    Grid origin (km)                 : (  -108.000, -1584.000)
    UTM zone                         :     0
    Grid cell width (km)             : (    36.000,    36.000)
    Number of cells                  : (  69,   67)
    Number of counties               :    96


    Layer AGL Ht (m)                 :        33.90 ( 1)
                                     :        84.90 ( 2)
                                     :       170.50 ( 3)
                                     :       256.80 ( 4)
                                     :       343.90 ( 5)
                                     :       431.70 ( 6)
                                     :       520.20 ( 7)
                                     :       609.50 ( 8)
                                            ... etc

    Species output list              :NO
                                     :NO2
                                     :OLE
                                     :PAR
                                     :TOL
                                     :XYL
                                     :FORM
                                      ... etc

 Number of records read from Vessel/Stack XREF file:       17

            Total Emissions Processed
                English Tons

                         NOX          CO          VOC
    -------------------------------------------------------
    Input Emissions      63.1642    112.3350      40.2407
    Output Emissions     63.1642    112.3350      40.2407
    Elevated Emissions    9.0931     12.0126       3.0029
    Surface Emissions    54.0711    100.3224      37.2378
    Outside Region        0.          0.           0.
    Written to ERR file   0.          0.           0.
    Total Skipped         0.          0.           0.
    -------------------------------------------------------
```

Exhibit 3-48. Example of a PSTSHP message file.

3.12 PSTPNT

In addition to a surface emissions file, the CAMx model requires a separate file containing elevated source emissions data. The EPS3 core system includes the PSTPNT (**P**o**ST**processor for elevated **P**oi**NT** source emissions) module, whose primary functions are

To create an ASCII stack list of elevated point sources,

To create an ASCII stack emissions file of elevated point sources, and

To provide the user with tabular summaries of elevated source emissions to assist in quality control tracking.

PSTPNT reads the EMBR file to extract the individual stack parameters and hourly emissions data for each elevated source. Only those EMBR records with a record type "E" (for "elevated") are written to the stack and emissions output files. PSTPNT is executed after all other processing of the point source data, prior to PIGEMS. In other words, PSTPNT should be the second to last module run for the point source emissions data.

PSTPNT also checks the state/county identification code (FIPS) on each input EMBR record against the user-supplied county list in the /COUNTY/ packet of the USERIN file. PSTPNT will write a warning message to the message output file if no EMBR records are found for a county listed in the /COUNTY/ packet.

Input Files

PSTPNT requires two input files: USERIN and an EMBR point source emissions file. PSTPNT reads five packets from USERIN:

/DATE/   This packet (Table 2-6) provides the modeling episode information.

/REGION/   PSTPNT uses this packet's data (Table 2-7) to determine if any points in the input EMBR file lie outside of the modeling domain. If such sources are encountered, they will be skipped.

/COUNTY/   PSTPNT reads this packet (Table 2-8) to check the county identification code specified on each input record against the region county list, and to determine if any counties from the region list had no corresponding EMBR data records.

/CRITERIA TABLES/ This packet (Table 2-11) specifies which criteria pollutant output tables, if any, the user wants to include in the output message file. See Section 2.4 for a full discussion on the output tables.

/SPECIES TABLES/ This packet (Table 2-11) specifies which chemical mechanism compound output tables, if any, the user wants to include in the output message file. See Section 2.4 for a full discussion on the output tables.

The second input file to PSTPNT is the EMBR file containing point source emissions data. The data in this file must be temporally allocated by hour (by the TMPRL module) and chemically speciated (SPCEMS or CHMSPL).

Output Files

PSTPNT creates five output files, two of which are required by the PIGEMS module, the final processing step for elevated point sources. PSTPNT creates a message file that summarizes elevated point source emissions by county (Exhibit 3-50). The first section of the message file summarizes input and output file names, region definition parameters, and the beginning and ending dates and times for the emissions data contained in the output file. The next section lists domain-wide totals of criteria pollutants and chemical mechanism compounds for both input and output emissions (including both low-level and elevated sources). The domain-wide totals may be followed by a series of warning messages indicating counties specified in the /COUNTY/ packet of USERIN for which no records were found in the input EMBR file. The final section provides emissions totals tables as specified in the USERIN packets, /CRITERIA TABLES/ and /SPECIES TABLES/.

The output stack list file contains the information needed to uniquely identify each stack, including FIPS, facility and stack identification codes, coordinates, and stack parameter information including stack height, exit temperature, diameter, exit velocity and flowrate (Exhibit 3-51). Stack parameter information is used to calculate plume rise (effective stack height) used in determining which layer the emissions from the source will be emitted.

The stack emissions file (Exhibit 3-52) contains the stack identifiers, stack parameters, coordinates,episode date, parent criteria pollutant name, air quality modeling compound name, and 24-hourly emission rates for each elevated point source. The output stack SCC file is an obsolete output file and should be left blank in the PSTPNT job script. The final output file is the EMAR error file that contains records that could not be processed.

Exhibit 3-49 shows an example of a PSTPNT job script.

```
#!/bin/csh
#
#    --- Sample job script for running the
#        EPS3 module PSTPNT
#
set EXEC = /models/eps3/src
#
set SCENARIO = test_problem
#
foreach DAY (wkd sat sun)
#
rm -f ../emiss/elvems.pts.$SCENARIO.$DAY
rm -f ../emiss/stkhdr.pts.$SCENARIO.$DAY
rm -f ../error/emar.pstpnt.pts.$SCENARIO.$DAY
rm -f ../msg/msg.pstpnt.pts.$SCENARIO.$DAY
#
echo "-------------------------------------------------"
echo "     Running PSTPNT for $SCENARIO - point sources"
echo "           Day - $DAY"
echo "-------------------------------------------------"

$EXEC/pstpnt/pstpnt << IEOF
USERIN file        :../inputs/userin.$SCENARIO.$DAY
Input EMBR file    :../embr/embr.tmprl.pts.$SCENARIO.$DAY
Output Messages    :../msg/msg.pstpnt.pts.$SCENARIO.$DAY
Output Emissions   :../emiss/elvems.pts.$SCENARIO.$DAY
Output Stack/HDR   :../emiss/stkhdr.pts.$SCENARIO.$DAY
Output Stack/SCC   :
EMAR error file    :../error/emar.pstpnt.pts.$SCENARIO.$DAY
IEOF
end
```

Exhibit. 3-49. Example of a PSTPNT job script.

```
          EPS3 PSTPNT module v. 1.01 Oct 2004      07/30/07 15:04:08

          Input Files
     USERIN file                    :../inputs/userin.test_problem.wkd
     Input EMBR file                :../embr/embr.tmprl.pts.test_problem.wkd

          Output Files
     Emissions file                 :../emiss/elvems.pts.test_problem.wkd
     Stack Header file              :../emiss/stkhdr.pts.test_problem.wkd
     STACKS/SCC file                : Not requested.
     ERROR file                     :../error/emar.pstpnt.pts.test_problem.wkd

               EPS3 PSTPNT module v. 1.01 Oct 2004      07/30/07 15:04:08

     File note                      :CAMx Modeling of Tx regional, 9/13/99
     Episode date (Calander)        :990913
     Episode date (Julian)          :99256
     Beginning hour                 :    0
     Ending hour                    :   24
     Grid origin (km)               : (  -108.000,  -1584.000)
     UTM zone                       :    0
     Grid cell width (km)           : (    12.000,    12.000)
     Number of cells                : (  135,  138)
     Number of counties             :   213

/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\

WARNING:   EMBR file contains stacks with matching ID but different stack parameters.
           County ID: 48001
           Plant ID: 0012
           Stack ID: 1
                     First Record     Second Record
           Diameter      0.7600           0.4600
           Height       16.8000          16.8000
           Exit Temp   620.0000         686.0000
           Exit Vel      7.1000          49.8000
           X-Coord     381.0670         381.0670
           Y-Coord    -873.7402        -873.7402
These records will be treated as separate stacks.
This is just the first occurance.  There may be others.

/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\

Total Emissions Processed
               English Tons

                    NOX          CO          VOC
     ------------------------------------------------------
     Input Emissions     2405.7701   1071.6300    646.8701
     Output Emissions    2084.9501    854.0600    172.2500
     Low Level Emissions  320.8200    217.5700    474.6200
     Written to EMAR         0.          0.          0.
     Emissions Skipped    320.8200    217.5700    474.6200
     ------------------------------------------------------
```

Exhibit 3-50. Example of a PSTPNT message file.

```
ORIGINAL    48001       0012        1                       16.8        0.460       686.    179280.     381067.     -873740.
ORIGINAL    48001       0012        1                       16.8        0.760       620.     25560.     381067.     -873740.
ORIGINAL    48001       0013        1                       22.6        0.980       700.     39600.     406681.     -879023.
ORIGINAL    48001       0013        1                       22.6        1.010       478.     54720.     406681.     -879023.
ORIGINAL    48005       0001        1                       22.9        2.260       339.     36360.     508081.     -933727.
ORIGINAL    48005       0001        1                       21.3        0.700       450.     51480.     508081.     -933727.
ORIGINAL    48005       0001        1                       21.3        1.580       319.     34560.     508081.     -933727.
ORIGINAL    48005       0002        1                       22.6        0.970       355.     53640.     508081.     -933727.
ORIGINAL    48005       0002        1                       20.1        0.800       355.     57240.     508081.     -933727.
ORIGINAL    48005       0002        1                       25.9        0.880       332.     92520.     508081.     -933727.
ORIGINAL    48005       0002        1                       36.6        1.970       341.     64080.     508081.     -933727.
ORIGINAL    48005       0002        1                       15.2        1.800       333.     24480.     508081.     -933727.
```
Exhibit 3-51. Example of stack header file created by PSTPNT and input to PIGEMS.

```
48001       0012        1                       16.8        0.460       686.    179280.     381067.    -873740. 990913 NOX
      0.040 NO                    15.120       15.120       15.120       15.120       15.120       15.120       15.120
15.120       15.120       15.120       15.120       15.120       15.120       15.120       15.120       15.120       15.120
      15.120       15.120       15.120       15.120       15.120       15.120       15.120
48001       0012        1                       16.8        0.460       686.    179280.     381067.    -873740. 990913 NOX
      0.040 NO2                   15.120       15.120       15.120       15.120       15.120       15.120       15.120
15.120       15.120       15.120       15.120       15.120       15.120       15.120       15.120       15.120       15.120
      15.120       15.120       15.120       15.120       15.120       15.120       15.120
48001       0012        1                       16.8        0.460       686.    179280.     381067.    -873740. 990913 VOC
      0.020 OLE                    3.493        3.493        3.493        3.493        3.493        3.493        3.493
3.493        3.493        3.493        3.493        3.493        3.493        3.493        3.493        3.493        3.493
      3.493        3.493        3.493        3.493        3.493        3.493        3.493
48001       0012        1                       16.8        0.460       686.    179280.     381067.    -873740. 990913 VOC
      0.020 PAR                   43.847       43.847       43.847       43.847       43.847       43.847       43.847
43.847       43.847       43.847       43.847       43.847       43.847       43.847       43.847       43.847       43.847
      43.847       43.847       43.847       43.847       43.847       43.847       43.847
48001       0012        1                       16.8        0.460       686.    179280.     381067.    -873740. 990913 VOC
      0.020 TOL                    0.049        0.049        0.049        0.049        0.049        0.049        0.049
0.049        0.049        0.049        0.049        0.049        0.049        0.049        0.049        0.049        0.049
      0.049        0.049        0.049        0.049        0.049        0.049        0.049
48001       0012        1                       16.8        0.460       686.    179280.     381067.    -873740. 990913 VOC
      0.020 XYL                    0.078        0.078        0.078        0.078        0.078        0.078        0.078
0.078        0.078        0.078        0.078        0.078        0.078        0.078        0.078        0.078        0.078
      0.078        0.078        0.078        0.078        0.078        0.078        0.078
```
Exhibit 3-52. Example of stack emissions file created by PSTPNT and input to PIGEMS.

3.13 PIGEMS

The PIGEMS (**P**lume-**I**n-**G**rid **EM**ission**S**) module serves two functions. First, it serves as the exit stage for the EPS3 system, producing an elevated emissions file for the CAMx photochemical model. Second, it provides a sophisticated methodology for flagging sources for the Plume in Grid (PiG) treatment within CAMx. Ultimately, the decision to simulate a point source plume with PiG is based on the emission rate of the source. Any source that emits at a rate greater than a user-specified threshold value will be flagged for the PiG treatment. The complexity of the PIGEMS module stems from two design elements:

1) flexibility in how threshold values can be assigned, and

2) ability to combine similar co-located sources into a single plume

> ➤ **Special Note**
> Although the execution of PIGEMS can be complicated, it can also be easily run to format elevated point source stack lists and emission files prepared by PSTPNT for input into the CAMx model. In this form, the PIGEMS module serves as tool for merging elevated point source files and reformatting for use with CAMx. See the "Running the PIGEMS Module" later in this section.

Flexible Emissions Threshold

It is often advantageous to apply a different threshold value for PiG sources based on criteria such as geographical location. For example, the sources contained in a small region of interest within the modeling domain could be selected for PiG using a lower threshold, producing a finer network of PiG sources in that area, without unnecessarily generating a multitude of PiG sources in the surrounding region. The PIGEMS module supports variable threshold values by allowing users to assign a threshold code. Associated with each threshold code is a pollutant name and an emissions value. Any source that emits the specified pollutant above the threshold rate will be flagged as a PiG source. Threshold codes are defined in the /THRESHOLD VALUE/ packet of the USERIN file found under the discussion of the PIGEMS inputs. Each source in the emissions inventory is then assigned to a threshold code. This assignment can be done in two ways, by county or by grid cell. The assignment of sources by grid cell is done via a "mask" file.

Combining Sources using Co-location

The simplest methodology by which to identify a source for the PiG treatment is to compare the emission rate of the source to the threshold value. However, this methodology would exclude clusters of similar, closely located sources from which individual plumes would merge to form a single plume such that the combined emission rate exceeds the threshold. For example, a facility could contain two stacks, standing tens of meters apart, each emitting at a rate that is two-thirds of the threshold value. Treated individually, neither of these stacks would be flagged for PiG. But combined as a single source, the pair easily exceeds the threshold. The process of combining multiple sources that are in close proximity to each other is defined as "co-location." The PIGEMS module determines co-located sources using the following steps:

1. Determine if the source is "significant" (defined as one-fourth of the threshold value). Sources that emit below this level are not considered.

2. Find all sources that are within a user-specified co-location distance. These are considered close enough to merge into a single common plume immediately after release. In order to avoid including a large number of small sources in a single cluster, sources that are deemed to be "insignificant" (less than 2.5% of the threshold) are ignored.

3. Compare the aggregate emission rate for sources in this cluster against the threshold value.

4. If the aggregate emission rate for the cluster exceeds the threshold value, a new source is created with the combined emission rate of the cluster, and this source is flagged for PiG treatment. The stack parameters of the new source will be an "average" of the stack parameters of all of the sources in the cluster. See the description of the stack parameter averaging presented later in this section.

5. Eliminate the sources in the cluster from consideration for co-location of other sources. This prevents a source from being included in multiple clusters, and thus potentially multi-counting that source's emissions.

The co-location of sources cannot be performed for multiple pollutants. Although it is possible to flag individual sources for PiG treatment according to either a NOx threshold value or a different VOC threshold value, the PIGEMS module can only co-locate multiple sources for PiG based on one pollutant. The name of the pollutant that is to be used as the co-location pollutant, as well as the co-location distance, is supplied in the /THRESHOLD VALUE/ packet of the USERIN file.

Combining a User-Defined Array of Sources

Co-locating sources is performed automatically and is determined strictly by proximity. However, there may be instances where it would be necessary to combine sources that would not be clustered using the co-location algorithm. For example, it may make sense to cluster a large array of small sources, such as in an oil or chemical processing facility, that are spread out over a fairly large area but act photochemically as a single plume from the facility. For this reason, the PIGEMS module allows for user-specified clusters. The user must provide newly created stack identification information (county code, facility ID and stack ID) for the new source, as well as the existing stack identification information for all of the sources that are to be combined to create this new source. Any existing stacks can be combined into a new source, although this only makes sense from a photochemical modeling standpoint for a few specific cases. Note that this feature should be used only after careful consideration of the possible impacts.

There is an option to specifically supply stack parameters and location coordinates of the newly created source, or have the PIGEMS module automatically average the values from the combined sources to create the stack parameters of the newly created source. To have the stack parameters and location coordinates automatically calculated, simply enter a missing value (-9) in the field for that parameter in the /COMBINE STACKS/ packet of the USERIN file. The /COMBINE STACKS/ packet is described in detail later in this section.

The Master Stack List

In many instances, point sources are processed using day-specific emissions in which some sources operate on a regular schedule (e.g., weekday/weekend), and others are used only occasionally (e.g., peaking units, etc.). If separate inventory processing streams are used for each day of a simulation period, this can lead to different point source lists day-to-day as various point sources shut down and others start up. In order to ensure that all point sources that will emit above the user-defined thresholds at some period in the simulation will receive the PiG treatment, it is necessary to have a single cohesive list of stacks for the inventory. This list, called the master stack list, must include any stack that emits at any time during the modeling period. For example, an auxiliary unit that emits at a rate that exceeds the threshold (and so should be flagged for PiG) may be active only during a weekend period. If PiG selection is applied only to the weekday emissions inventory files, this source would be skipped. The simple solution is to run PiGEMS for each day in the episode. However, this could lead to a series of independent PiG point source emissions files, each having a different list and order of stacks. While CAMx can accept such inconsistent PiG inputs (even if OSAT is invoked), these inconsistencies can lead to difficulties with database management.

The PIGEMS module handles this complication by first creating and then utilizing a master stack list. The first application of the PIGEMS module to an inventory should be performed to create a master stack list over all simulation days. When creating the master stack list, the PIGEMS module will also identify all of the sources that should be flagged for PiG treatment and put those sources at the top of the list. It will also identify any clusters via co-location, or user-defined stack combination, and create records in the master stack list for the newly created stacks. The master stack list is an ASCII file and can be edited to override the automatic assumptions made by the PIGEMS module. Once the master stack list is created, the PIGEMS module can be run again to create an emissions inventory file for each specified day of the inventory. The emissions inventory file will contain the entire complement of sources in the master stack list, including sources that do not emit on the given day.

RUNNING THE PIGEMS MODULE

Because of its flexibility and dual purpose nature – creating a master stack list or creating a model ready emissions file – the PIGEMS module job stream can be a bit daunting to configure. Some files are always needed; others should only be supplied under certain conditions. What follows are a few examples of PIGEMS run scripts, demonstrating how the module should be configured for a few of the typical scenarios.

Running PIGEMS When No PiG Treatment Is Needed

When no PiG is being performed by the photochemical model, the PIGEMS module acts as a simple reformatting program, with the added ability to merge files generated by separate EPS3 streams. Because of their consistent format, a stack definition file output by PSTPNT can be used as a master stack list input to the PIGEMS module. To ensure that all stacks are included in the inventory it is necessary to concatenate each of the stack definition files into a single stack definition file.

Exhibit 3-53 shows a sample job script for running the PIGEMS module when no PiG treatment is needed. In this case, it is not necessary to include any of the PIGEMS specific packets of the USERIN file. If these packets are included, they will be ignored. The output from this run of the PIGEMS module is a model-ready emissions file that contains all of the sources but represents

one day of the episode.

```
#!/bin/csh
#
#    --- Sample job script for running the
#        EPS3 module PIGEMS
#
set EXEC = /models/eps3/src
#
set SCENARIO = test_problem
#
foreach DAY (wkd sat sun)
#
rm -f ../msg/msg.pigems.$SCENARIO.$DAY
rm -f ../emiss/ptsrce.$SCENARIO.$DAY.bin
#
echo "-------------------------------------------------"
echo "    Running PIGEMS for $SCENARIO - point sources"
echo "         Day - $DAY"
echo "-------------------------------------------------"

$EXEC/pigems/pigems << IEOF
USERIN file         :../inputs/userin.$SCENARIO.$DAY
Master Stack List  : ../emiss/stkhdr.pts.$SCENARIO.$DAY
No Stack def. file :/END/
Stack emiss files  : ../emiss/elvems.pts.$SCENARIO.$DAY
                     /END/
Threshold Mask file:
Message file        :../msg/msg.pigems.$SCENARIO.$DAY
Output Master Stack:
Output Emissions   :../emiss/ptsrce.$SCENARIO.$DAY.bin
IEOF
end
```

Exhibit 3-53. Example of a PIGEMS job script, when no PiG treatment is needed.

Running PIGEMS to Create The Master Stack List

To create the master stack list, both the full complement of stack definition files and the full complement of stack emissions files must be supplied to the PIGEMS module. All of the stack definition files, including all days, must be supplied so that the master stack list includes each stack that emits at any time during the modeling episode. The PIGEMS module ignores repeated instances of stacks, creating a stack list that contains a single entry for each stack. All of the stack emissions files, including all days, must be supplied so that the PIGEMS module can determine if any stack emits at a rate that exceeds the threshold at any time during the modeling episode. Obviously, a valid filename must be supplied for the output master stack list, but it is important that the filename for the input master stack list is left blank. Exhibit 3-54 shows an example of a job script configured for the PIGEMS module to **create** a master stack list.

```
#!/bin/csh
#
#  Script to run PIGEMS to create master stack list
#
#=============================================================================
#         Run PIGEMS to Create the Master Stack List
#=============================================================================
#
rm -f ../msg/msg.pigems.ext_reg.nei99v3.master_stacklist
rm -f ../emiss/master.stacklist.ext_reg_nei99v3
#
../../src/pigems/pigems.pts << ieof
USERIN file       :../inputs/userin.ext_reg.990813
Master Stack List :
No Stack def. files:../emiss/stkdef.pt.TX.egu_99po.990813
                   :../emiss/stkdef.pt.TX.egu_99po.990814
                   :../emiss/stkdef.pt.TX.egu_99po.990815
                   :../emiss/stkdef.pt.TX.egu_99po.990816
                   :../emiss/stkdef.pt.TX.egu_99po.990817
                   :../emiss/stkdef.pt.TX.egu_99po.990818
                   :../emiss/stkdef.pt.TX.egu_99po.990819
                   :../emiss/stkdef.pt.TX.negu_99po.sat
                   :../emiss/stkdef.pt.TX.negu_99po.sun
                   :../emiss/stkdef.pt.TX.negu_99po.wkd
                   :../emiss/stkdef.ext_reg.others_nei99v3.sat
                   :../emiss/stkdef.ext_reg.others_nei99v3.sun
                   :../emiss/stkdef.ext_reg.others_nei99v3.wkd
 /END/
 Stack emiss files :../emiss/stkemis.pt.TX.egu_99po.990813
                   :../emiss/stkemis.pt.TX.egu_99po.990814
                   :../emiss/stkemis.pt.TX.egu_99po.990815
                   :../emiss/stkemis.pt.TX.egu_99po.990816
                   :../emiss/stkemis.pt.TX.egu_99po.990817
                   :../emiss/stkemis.pt.TX.egu_99po.990818
                   :../emiss/stkemis.pt.TX.egu_99po.990819
                   :../emiss/stkemis.pt.TX.negu_99po.sat
                   :../emiss/stkemis.pt.TX.negu_99po.sun
                   :../emiss/stkemis.pt.TX.negu_99po.wkd
                   :../emiss/stkemis.ext_reg.others_nei99v3.sat
                   :../emiss/stkemis.ext_reg.others_nei99v3.sun
                   :../emiss/stkemis.ext_reg.others_nei99v3.wkd
                    /END/
Threshold Mask file:../inputs/pigems.maskfile.4km
Message file       :../msg/msg.pigems.ext_reg.nei99v3.master_stacklist
Output Master Stack:../emiss/master.stacklist.ext_reg_nei99v3
Output Emissions   :
ieof
```

Exhibit 3-54. Example of a PIGEMS job script. This is used to create a master stack list.

Running PIGEMS to Create a Model Ready Emissions File

Once the master stack list is created, the PIGEMS module can be run to create model-ready emissions files. A PIGEMS run must be made for each day of the modeling episode. In this configuration, the master stack list created in the previous run is used as the input stack list and only the stack emissions files for the day of interest are included. The lines containing the output master stack list and the threshold map file are ignored, as are the PIGEMS specific packets of the USERIN file. Exhibit 3-55 shows a job script for creating model-ready emissions files using the PIGEMS module. Notice that this script has a loop that walks through each day of the inventory.

```
#!/bin/csh
#
#  Script to run PIGEMS to create model-ready files
#
# --- loop over all days in the episode ---
#
foreach f (13.wkd 14.sat 15.sun 16.wkd 17.wkd 18.wkd)
#
#==========================================================================
#          Run PIGEMS to Create Model-Ready File
#==========================================================================
#
set cal = $f:r
set rep = $f:e
#
rm -f ../msg/msg.pigems.PiG.ext_reg.nei99v3.9908$cal
rm -f ../emiss/ptsrce.PiG.ext_reg_nei99v3.9908$cal.bin
#
echo '--------------------------------'
echo "        Doing Aug $cal"
echo '--------------------------------'
#
../../src/pigems/pigems.pts << ieof
USERIN file         :../inputs/userin.ext_reg.9908$cal
Master Stack List   :../emiss/master.stacklist.ext_reg_nei99v3
No Stack def. files:/END/
Stack emiss files   :../emiss/stkemis.pt.TX.egu_99po.9908$cal
                    :../emiss/stkemis.pt.TX.negu_99po.$rep
                    :../emiss/stkemis.ext_reg.others_nei99v3.$rep
                     /END/
Threshold Mask file:
Message file        :../msg/msg.pigems.PiG.ext_reg.nei99v3.9908$cal
Output Master Stack:
Output Emissions    :../emiss/ptsrce.PiG.ext_reg_nei99v3.9908$cal.bin
ieof
end
```

Exhibit 3-55. Example of a PIGEMS job script, to create the PiGged model ready files for each day in the inventory.

Running PIGEMS to Insert Additional Sources

Sometimes it is necessary to insert new sources into an inventory after all of the main processing has been completed. For example, on certain days of the episode in which a considerable number of wildfires added to the air quality problem, it may be necessary to insert the wildfire emissions, which have been processed as point sources. Or perhaps a future year control strategy calls for a new unit, which was not included in the standard processing, to be included in the inventory. The PIGEMS module allows for additional sources to be inserted when creating a model-ready emissions file. The new sources will be added to the list of sources and included in the inventory, but will not be considered for PiG treatment. The sources can be flagged for PiG treatment by manually changing the stack diameter field on the stack definition record to a negative value. To insert additional sources in the inventory, merely supply the PIGEMS module with an input master stack list and any number of stack definition files. Of course, the stack emissions files for the additional sources must also be supplied. Exhibit 3-56 shows an example of how to configure the PIGEMS module to insert additional sources for one day of the episode. In this example, a file containing wildfire emissions modeled as point sources is inserted.

```
#!/bin/csh
#
#  Script to run PIGEMS to create model-ready file
#  On this day there were wild-fires (which should
#  not be PiGged)
#
#===============================================================================
#          Run PIGEMS to Create PiGged PTSRCE file for Aug 15 (Sunday)
#===============================================================================
#
rm -f ../msg/msg.pigems.PiG.ext_reg.nei99v3.990815
rm -f ../emiss/ptsrce.PiG.ext_reg_nei99v3.990815.bin
#
../../src/pigems/pigems.pts << ieof
USERIN file        :../inputs/userin.ext_reg.990815
Master Stack List  :../emiss/master.stacklist.ext_reg_nei99v3
Additonal Stack def:../emiss/stkdef.fires.990815
                   /END/
Stack emiss files  :../emiss/stkemis.pt.TX.egu_99po.990815
                   :../emiss/stkemis.pt.TX.negu_99po.sun
                   :../emiss/stkemis.ext_reg.others_nei99v3.sun
                   :../emiss/stkemis.fires.990815
                   /END/
Threshold Mask file:
Message file        :../msg/msg.pigems.PiG.ext_reg.nei99v3.990815
Output Master Stack:
Output Emissions   :../emiss/ptsrce.PiG.ext_reg_nei99v3.990815.bin
ieof
```

Exhibit 3-56. Example of a PIGEMS job script, to add additional sources to the inventory.

Input Files

The PIGEMS program anticipates five input files: the USERIN file, the master stack list, stack definition files, stack emissions files, and an optimal threshold mask file. The input master stack list is blank if the PIGEMS run is to create the list. The stack definition files are optional if an input master stack list is provided.

USERIN File

The PIGEMS module reads four of the standard USERIN packets and an additional three packets specific to PIGEMS.

/DATE/   This packet (Table 2-6) provides the modeling episode information.

/REGION/   This packet (Table 2-7) provides the region definition and is used to convert source locations to grid cell.

/CRITERIA POLLUTANT/ PIGEMS reads this packet (Table 2-9) to determine which of the input pollutants to include in the modeling inventory. .

/SPECIES LIST/ This packet (Table 2-11) provides the air quality model species list.

All of the PIGEMS-specific packets are optional, although failing to supply either the /THRESHOLD VALUE/ or the /THRESHOLD MAP/ packets will result in the inability of the PIGEMS module to flag any sources for PiG treatment. Therefore, when processing an inventory for a photochemical modeling application in which the Plume-in-Grid sub-model will not be used, the THRESHOLD packets are not required.

/THRESHOLD VALUE**/** This packet contains the threshold values that will be used to determine if a source is to be flagged for PiG. The first record of this packet contains the co-location information: specifically, the co-location distance and the co-location pollutant (Table 3-34). The co-location distance is the distance (in meters) that the PIGEMS module will use to determine if a group of stacks forms a cluster. The emissions from stacks that are within this distance of one another will be aggregated to determine if the combination exceeds the threshold. Because a different threshold value can be supplied for each pollutant, the PIGEMS module also needs to be provided the name of the pollutant that is to be used for purposes of co-location. This is referred to as the co-location pollutant. Only threshold values associated with this pollutant will be used when determining the co-located sources.

The remaining records of the /THRESHOLD VALUE/ packet contain the threshold codes and the associated threshold value (in tons per day), as well as the name of the pollutant to which the threshold applies. The threshold code must be an integer between 1 and 99. The same threshold code could be used for multiple pollutants. If a source is mapped to this threshold code then it will be flagged for PiG treatment if either of the threshold values is exceeded. For example, suppose there is a record with a threshold code of 1 that has a NOx threshold of 50 tons per day. Also suppose there is a record with threshold code 1 but with a VOC threshold of 10 tons per day. If a source (or a cluster of sources) emits over 50 tons per day of NOx *or* 10 tons per day of VOC it will be flagged for PiG. Table 3-34 shows the format of the /THRESHOLD VALUE/ packet. Exhibit 3-57 shows a sample /THRESHOLD VALUE/ packet.

Table 3-34. The /THRESHOLD VALUE/ packet.

Variable	Columns	Description
	1 – 20	Ignored, used for notational purposes.
Colodist	21 – 30	Co-location distance (m)
Colocpol	31 – 40	Pollutant for which co-location is based.
ithrshcd( )	21 – 30	Numeric code for threshold (1-99)
Thrshspc( )	31 – 40	Criteria pollutant code for which the threshold applies.
thrshval( )	41 – 50	Threshold value for corresponding code and pollutant.

```
   /THRESHOLD VALUE/
   coloc dist, poll   : 250.          NOX
   id, specie, val    : 1            NOX      20.
   id, specie, val    : 2            NOX      50.
   /END/
```

Exhibit 3-57. Sample /THRESHOLD VALUE/ packet. This packet could be used to apply a more stringent threshold to an area of interest.

/THRESHOLD MAP/ This packet is used to assign a threshold code to sources based on the county in which they are contained. Each record defines one mapping, by defining a state/county FIPS code and the threshold code to which that county is to be assigned. The threshold code must be listed in the /THRESHOLD VALUE/ packet where the actual threshold value will be defined. The regular EPS3 best-match criteria will be applied to the FIPS codes for purposes of matching sources. For example, a code of 06067 will be a better match than a code of 06000. Because all sources should have some threshold code mapping, it is important to have a record in this packet with the "catch-all" FIPS code of 00000. If this is not included some sources may not have a threshold code mapping and will not be considered for PiG treatment. Table 3-35 shows the format of the /THRESHOLD MAP/ packet, while Exhibit 3-58 shows an example.

Table 3-35. The /THRESHOLD MAP/ packet.

Variable	Columns	Description
	1 - 20	Ignored, used for notational purposes.
thrshcty( )	21 - 30	County code for which threshold applies.
ithrshmap( )	31 - 40	Numeric code for threshold value (corresponds to code specified in /THRESHOLD VALUE/ packet).

```
   /THRESHOLD MAP/
   All counties       : 00000      2
   Texas counties     : 48000      1
   /END/
```

Exhibit 3-58. Sample /THRESHOLD MAP/ packet. This packet could be used to apply a more stringent threshold to an area of interest.

/COMBINE STACKS/ This packet allows any user-defined set of stacks to be combined into a single stack. This facilitates the clustering of sources that would not normally be combined using the automated co-location algorithm. This packet is comprised of a set of records, each set defining the new stack's characteristics as well as identifying the existing stacks that will be combined. The format of the packet records (Table 3-36) is the same as the records in the stacks definition file produced by the PSTPNT module and the master stack list processed by the PIGEMS module. This means populating a /COMBINE STACKS/ record can be done by extracting the records of the stacks to be combined from the existing stack definition file and then creating a new stack definition record for the newly created source. Note that the new stack definition record is similar to the existing stack definition records but has an additional field for determining if the newly created stack should be considered for PiG treatment. It may be useful to combine stacks without applying the PiG treatment and the /COMBINE STACKS/ allows for this.

Because the record identifying the new source must have unique stack identification information, it is important to come up with a coding scheme that will yield a unique stack ID. For example, the string NEWSTK0001 could be used for the new stacks, incrementing the numeric portion for each new stack. The county code and facility identification codes should be taken from the sources being combined. The keyword at the beginning of the record should be the word "NEW" for the new stack definition record, and a blank string for those records listing the sources to be combined. When combining stacks defined in the /COMBINE STACKS/ packet, the PIGEMS module will either use the stack parameters listed on the new stack record or, alternatively, "average" the stack parameters of the stacks to be combined. To force the use of the averaging scheme the stack parameters on the new stack record should be set to missing value (-9.0). When "averaging" stack parameters of combined stacks, the PIGEMS module will follow this algorithm:

1. Average the coordinates,
2. Average the volumetric flow rates,
3. Calculate the square root of the sum of the squares of the diameter,
4. Calculate the maximum stack height,
5. Calculate the average of the exit temperatures weighted by the volumetric flow rate,
6. Calculate the gas exit velocity from the newly calculated volumetric flow rate and diameter.

This is also the averaging scheme that is used when combining sources that are automatically co-located. Exhibit 3-59 provides an example of the /COMBINE STACKS/ packet.

Table 3-36. The /COMBINE STACKS/ packet.

Variable	Columns	Description
The following refers to the new stack record. This record is followed by a series of existing stack records, one for each existing stack to combine.		
keyin	1 - 10	Keyword 'NEW' for new stack definition followed by keyword 'PIG' or 'NOPIG' indicator.
ctynew( )	12 - 21	County code for the new stack.
facnew( )	23 - 32	Facility ID for new stack
stidnew( )	34 - 43	Stack ID for new stack
hgtnew( )	45 - 54	Stack height for new stack (negative value indicates to calculate from combined stacks) (m)
dianew( )	56 - 65	Stack diameter for new stack (m)
tptnew( )	67 - 76	Stack gas exit temperature for new stack (K)
velnew( )	78 - 87	Stack gas exit velocity for new stack (m/s)
xlocnew( )	89 - 98	X-coordinate for new stack
ylocnew( )	100 - 109	Y-coordinate for new stack
The following refers to the existing stack record. These records are the same format as the stack definition file(output of PSTPNT) and the master stack list. There will typically be multiple instances of this record for each new stack record.		
	1 - 10	Blank indicates stack to be combined
ctycomb( )	12 - 21	County code for stack to combine to create new stack
faccomb( )	23 - 32	Facility ID for stack to combine to create new stack
stidcomb( )	34 - 43	Stack ID for stack to combine to create new stack

```
 /COMBINE STACKS/
 NEW PIG     01001      1         NEWSTK0001      -9.0      -9.0      -9.0       -9.0       -9.0      -9.0
             01001      1         001
             01001      1         002
             01001      1         003
 NEW NOPIG   01073      7         NEW0000002      215.5     7.620     433.      90720.    1176037.   -596587.
             01073      7         001             213.4     7.620     433.      90720.    1176037.   -596587.
             01073      7         002             213.4     7.620     409.      73800.    1176037.   -596587.
             01073      7         004             213.4     7.620     411.      81360.    1176037.   -596587.
             01073      7         005             215.5     7.620     409.      80280.    1176053.   -596685.
             01073      7         005
 /END/
```

Exhibit 3-59 Sample /COMBINE STACKS/ packet. (Notice that since only the first 3 fields of the records containing the stacks to combine are read, the later fields can be included, but they will be ignored.)

The Input Master Stack List

This file contains the list of all sources that will emit at any time during the episode period. The PiG sources will appear at the top of the file. The format of the master stack list is identical to the format of the stacks definition file (Table 3-37) produced by the PSTPNT module. Therefore, for an application in which the PiG treatment is not needed it is possible to supply the PSTPNT-produced stack definition file to the PIGEMS module as the master stack list. The result will be a model ready emissions file with no sources flagged for PiG. In the likely event that the EPS3 processing produced multiple PSTPNT stack definition files (by source category, for example) it is necessary to concatenate the stack definition files from the separate EPS3 streams. Since the PSTPNT stack definition file is an ASCII file with one record for each stack, this can be done using the Unix "cat" command, followed by the "sort –u" command to generate a unique list of stacks.

The PIGEMS module will typically be executed several times. The first run, which is significantly different from the standpoint of input file requirements than succeeding runs, is performed to create the master stack list. In this instance, the input master stack list filename should be left blank. This tells the PIGEMS module that a master stack list should be created, in which case an output master stack list should be supplied. If both an input master stack list file and an output master stack list file are supplied it is assumed that the input master stack list is valid and the PIGEMS module will ignore the line containing the name of the output master stack list. Subsequent runs of the PIGEMS module produce model-ready inventory files for each of the days of the modeling episode. In this instance, the master stack list file produced during the first execution of the PIGEMS module should be supplied as the input master stack list.

Table 3-37. Stack definition file format.

Variable	Columns	Description
Keywrd	1 – 10	Keyword; ORIGINAL
Ctytmp	12 – 21	County FIPS code
Factmp	23 – 32	Facility identifier
Stktmp	34 – 43	Stack identifier
Hgttmp	45 – 54	Stack height (m)
Diatmp	56 – 65	Stack diameter (m)
Tpttmp	67 – 76	Stack exit gas temperature (K)
Veltmp	78 – 87	Stack exit gas velocity (m/s)
Xloctmp	89 – 98	Stack X location
Yloctmp	100 – 109	Stack Y location

The Input Stack Definition Files

The PIGEMS module accepts an indeterminate number of PSTPNT-produced stack definition files. These must be supplied when creating a master stack list, but also can be used to add additional sources to an inventory. For example, a user may want to add a list of permitted, but not yet constructed sources, as a sensitivity run. When supplied both an input master stack list and additional input stack definition files, the PIGEMS module will simply add the sources contained in the stack definition files to the list of sources from the master stack list to include them in the inventory. Be aware that when adding sources to an inventory in this way, the additional sources will not be flagged for PiG treatment. When creating a master stack list, all of the stack definition files from the separate PSTPNT runs must be supplied, including the stack definition files for the different episode days and from different source category streams. The PIGEMS module will ignore the duplicates and create a stack list that contains all of the sources, apply the various criteria for application of PiG treatment, and write out a comprehensive master stack list. To supply multiple input stack definition filenames, simply list each file on a separate line and terminate the list with the keyword /END/ in place of a filename (Exhibit 3-54).

The Input Stack Emissions Files

Like the stack definition files, the stack emissions files (Table 3-38) are produced by the PSTPNT module. One stack emissions file will be produced for each EPS3 stream. Unlike the stack definition files, a set of stack emissions files must be supplied each time the PIGEMS module is utilized. When creating a master stack list, the PIGEMS module needs access to the entire complement of stack emissions files, including all days in the episode. This is necessary for the PIGEMS module to determine if a source (or source cluster) exceeds the threshold on any

day during the entire episode. The PIGEMS module merely calculates the maximum daily emissions for each source and uses this value to compare against the threshold value for purposes of flagging sources for PiG treatment. When running the PIGEMS module to produce a model-ready emissions file for point sources it is only necessary to supply the emissions files for that day of the episode.

Table 3-38. PSTPNT emissions output file format.

Variable	Columns	Description
ctytmp	1 – 10	County FIPS code
factmp	12 – 21	Facility identifier
stidmp	23 – 32	Stack identifier
hgttmp	34 – 43	Stack height (m)
diatmp	45 – 54	Stack diameter (m)
tpttmp	56 – 65	Stack exit gas temperature (K)
veltmp	67 – 76	Stack exit gas velocity (m/s)
xloctmp	78 – 87	Stack X location of (x,y) convention
yloctmp	89 – 98	Stack Y location of (x,y) convention
	100 - 105	Inventory date
	107 - 116	Criteria pollutant code
	118 - 127	Daily emissions estimates for criteria pollutant (tons/day)
spctmp	129 - 138	Speciated pollutant code
emsval( )	140 - 149	Emission estimates for speciated pollutant for hours 1 through 24
	151 - 160	(moles/hour)

During EPS3 processing it is often the case that a representative day inventory file is generated, rather than a specific-day inventory file. For example, it is typical to produce just a single file representing all weekdays in the summer season, rather than the dozens of files that would account for weekdays during this period. For this reason, the PIGEMS module does not perform any date matches when processing the emissions files. Therefore, it is critical to ensure that the list of stack emissions files supplied to the PIGEMS module represents a single day inventory that is complete. All of the emission records for a given stack will be added to the total emissions for the stack. To terminate the list of emissions files in the job script of the PIGEMS module, include the /END/ keyword in place of a filename.

The Threshold Mask File

The optional threshold mask file is used to define the threshold value for sources based on the grid cell in which the source is located. The mask file is essentially a map of the modeling domain in which each modeling grid cell is assigned a number, called the threshold code, representing the threshold value to be applied to that cell. The origin of the modeling domain, defined in the /REGION/ packet of the USERIN file, appears as the lower left-hand corner of the mask file, so that when viewing the file in an editor it looks like the modeling domain, easting moving from left to right and northing moving from bottom to top. The threshold code, which is an integer, appears in a field of 3-characters.

Because political boundaries are more precise in identifying sources than modeling grid cells, any assignment in the /THRESHOLD MAP/ packet that is not the global county code (00000) will override the assignment in the mask file. For example, suppose a source in Sonoma County, CA is assigned a threshold code of 1 using the threshold mask file. If the only match for Sonoma County in the /THRESHOLD MAP/ packet is the global county code 00000, the mask file will

file will take priority. However, if the /THRESHOLD MAP/ packet contains a state FIPS code for California (06000) or the specific Sonoma County FIPS code (06097), the assignment from the /THRESHOLD MAP/ packet will be used. Exhibit 3-60 shows an example of the threshold mask file.

```
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
     .
     .
     .
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 2 2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 2 2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 2 2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

Exhibit 3-60. Sample Threshold Mask File.

Output Files

PIGEMS Message File

The PIGEMS module generates a standard EPS3 message file. This file contains a history of the run, including the date and time of the execution, a list of input and output files used and the user parameters specified in the USERIN file. The message file also contains one of two tables for QA purposes. The first table contains a count of the stacks in each input stack definition file and the second table contains the emissions totals for the stacks processed, also separated by input file. In each case, the information is reported by the following categories:

1. Total number of stacks.
2. Number of stacks that were flagged for PiG treatment.
3. Number of stacks identified for co-location.
4. Number of stacks combined using user definition.
5. Number of stacks in which the mask file determined the threshold code.

When running the PIGEMS module to produce a master stack list, only the table of stack counts will be produced. Alternatively, only the table of emissions totals will be produced when running the PIGEMS module to produce a model-ready emissions file. Exhibit 3-61 shows a PIGEMS message file.

```
                 EPS3 PIGEMS module v. 1.2 Aug 2005        07/25/07 18:43:38

            Input Files
        USERIN file                     :../inputs/userin.test_problem.wkd
        Input master stack list file  :../emiss/stkhdr.pts.test_problem.wkd
        Input stack emissions files
        Emiss file 001                  :../emiss/elvems.pts.test_problem.wkd
        Threshold mask file             : Not provided.

            Output Files
        Using Input Master stack list : No output master stack list will be
                                            created.
        Emissions file                  :../emiss/ptsrce.test_problem.wkd.bin

                 EPS3 PIGEMS module v. 1.2 Aug 2005        07/25/07 18:43:38

        File note                       :CAMx Modeling of Tx regional, 9/13/99
        Episode date (Calander)         :990913
        Episode date (Julian)           :99256
        Beginning hour                  :    0
        Ending hour                     :   24
        Grid origin (km)                : (  -108.000, -1584.000)
        UTM zone                        :    0
        Grid cell width (km)            : (    12.000,    12.000)
        Number of cells                 : (  135,  138)

        Colocation dist (m)             :     0.00000


        Threshold Code Values read from USERIN file.
            Code    Species    Level (tons/day)


        Threshold Code Mappings read from USERIN file.
            FIPS Code    Threshold Code

             Table of Emissions Processed


        Input File            NOX          CO         VOC
     -----------------------------------------------------------
     Emiss file 001        2084.4503    852.5801    154.3051
     -----------------------------------------------------------
     Total                 2084.4502    852.5801    154.3051
```

Exhibit 3-61. Example of a PIGEMS message file.

Output Master Stack List File

This filename must be supplied when running the PIGEMS module to produce a master stack list. The PIGEMS module decides whether it should create a master stack list by looking at the filename for the input master stack list. If this filename is a blank string it is assumed that a master stack list is to be produced, in which case the line in the job script containing the output master stack list must contain a valid filename. However, if a valid filename is supplied for the input master stack list, it is assumed that a model-ready emissions file is to be produced and the line containing the output master stack list filename is ignored. The format of the output master stack list is the same as the stack definition files produced by the PSTPNT module.

Output Emissions File

This file is a binary model-ready point source emissions file containing a single day of hourly emissions for each of the stacks in the inventory. It is produced when running the PIGEMS module where an input master stack list is provided. When running the PIGEMS module to produce a master stack list, .i.e. the input master stack list file is blank and the output master stack list file is valid, this file is ignored.

3.14 GRDEM

The GRDEM (**GRiD EM**issions) module allows the user to spatially allocate emissions to the grid cells of the modeling domain. The GRDEM module will

Spatially allocate county level area and mobile sources based on gridded spatial surrogates or (optional) digitized links,

Assign low-level point source emissions to grid cells based on source location, and

Create either a gridded EMBR or CAMx model-ready surface emissions file.

For area sources, GRDEM spatially allocates emissions (e.g., county-level or subregion-level emissions) by source category based on the spatial apportionment surrogate for that source category as specified in the SCC(ASC)/gridded surrogate cross-reference file. Each source category is mapped to a spatial surrogate (a quantity whose areal distribution is either known or has been estimated and is assumed to be similar to the areal distribution of emissions from some source category whose spatial distribution is unknown.) Examples of commonly used gridded surrogates are population and urban landuse.

Because the databases used to create gridded surrogates (such as land use coverages) can be incomplete, there are sometimes "holes" in a given gridded surrogate field. This will cause an artificial loss in emissions. To handle this problem, GRDEM supports the assignment of 3 surrogate codes to each source category code; a primary, a secondary and a tertiary code. The GRDEM module will check the gridded surrogate fields for a given county to ensure that the field assigned as the primary surrogate for a given source category is complete (that is, the entire county has been gridded). If it is incomplete the GRDEM module will then check the secondary surrogate field for completeness. If this is not complete, the GRDEM module will default to using the tertiary code. Since the tertiary code is the last chance, it is recommended that this surrogate be derived from a reliable database, such as total land area. To use the secondary and tertiary codes, the GRDEM module must be able to verify the completeness of the surrogate fields. This requires that each county in the modeling domain be completely gridded. To accomplish this, it is sometimes necessary to extend the landuse coverages past the edges of the modeling domain; to ensure that an entire county is covered by surrogate data. To avoid this requirement, turn off the secondary and tertiary codes option in the /GRDEM/ packet of the USERIN file.

If digitized link data are available for some categories (e.g., light-duty automobiles on limited access roadways, railroad locomotives, shipping vessels), GRDEM will determine the cells traversed by each link and allocate emissions for that source category accordingly. Alternatively,

the user may specify that emissions from these sources be allocated based on a spatial surrogate. Note the distinction between link-based emissions, which are processed by the LBASE module and include the effects of varying activity levels for each link, and spatial allocation of emissions using link data, in which county-level emissions are allocated evenly along all links of that type within the county based solely on the length of the link. For low-level point sources, GRDEM assigns emissions to grid cells based on the geographical coordinates of the source.

GRDEM will write a surface emissions file in either EMBR format or the format used by the air quality model. If EMBR format is chosen, GRDEM will fill in the cell index fields in each output EMBR record. If the CAMx format is chosen, the input EMBR file must be hourly and have the chemical resolution required by the model. Generally this means TMPRL and SPCEMS or CHMSPL modules must have already been run. For the input invnetiories that are provided at hourly resolution TMPRL need not be run.

If GRDEM encounters an input record in which the grid cell field has previously been filled in (that is, an EMBR record that has already been gridded), it writes the record as-is to the output file if EMBR output has been specified. If the CAMx format has been specified, GRDEM combines the emissions for that source with the other surface emissions in that grid cell. Processing then continues at the next input record.

Input Files

GRDEM uses five input files: the USERIN file, an EMBR emissions file, the file cross referencing SCC (ASC) codes and surrogate spatial allocation codes, a file containing the distribution of the surrogate data in the modeling grid, and an optional file containing definitions of transportation links.

GRDEM reads the following packets from USERIN:

/GRDEM/ This packet (Table 3-39 and Exhibit 3-62) contains two parameters. The first is a flag specifying the format of the output emissions file; "YES" indicates CAMx-format, and "NO" indicates EMBR format. The second parameter is the flag for using the secondary and tertiary surrogate codes. If set to "YES" GRDEM will implement the secondary and tertiary codes. If this flag is set to "NO", GRDEM will only read and utilize the primary surrogate codes.

Table 3-39. /GRDEM/ packet of EPS3 global user input file, USERIN.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	C	Packet identifier = /GRDEM/
2		1-20		Not used
	CAMXFLG	21-30	C	Flag for output in model emissions file format: YES = output is CAMX format NO = output is EMBR format COMP = compressed, criteria only EMBR for SPLTEM utility
3		1-20		Not used
	LALTSRG	21-30	C	Use secondary and tertiary codes: YES = use all 3 codes NO = use primary code only
4	KEYEND	1-20	C	Packet terminator = /END/

```
/GRDEM/
Output is CAMx    : YES
Use Secondary Surgs: NO
/END/
```

Exhibit 3-62. GRDEM packet of USERIN

/SPECIES LIST/ GRDEM reads this packet of the user input file (Table 2-11) in order to obtain the species list.

/DATE/   GRDEM reads the dates of the modeling episode from this packet (Table 2-6).

/REGION/   GRDEM reads this packet (Table 2-7) to determine the size and configuration of the modeling domain grid.

/COUNTY/ This packet contains the list of counties within the modeling domain (Table 2-8).

/CRITERIA TABLES/ This packet (Table 2-11) specifies which criteria pollutant output tables, if any, the user wants to include in the output message file. See Section 2.4 for a full discussion on the output tables.

/SPECIES TABLES/ This packet (Table 2-11) specifies which chemical mechanism compound output tables, if any, the user wants to include in the output message file. See Section 2.4 for a full discussion on the output tables.

The second input file, the EMBR emissions file, can contain data at any stage of EPS3 processing (in other words, the GRDEM module may be run at any point in the process after PREPNT, PREAM, or LBASE). Due to the size of the gridded EMBR files created by GRDEM, however, it is advisable to run the GRDEM module last (i.e., after all other processing of that particular set of data has been completed). When GRDEM is run last, select the "YES" option for CAMx format output.

The third input file contains the SCC(ASC)/spatial surrogate cross-reference table that allows the user to tailor the distribution of emissions for a particular region (Table 3-40 when using secondary surrogate codes, Table 3-41 when using only primary codes). In this file each SCC(ASC) code is assigned a spatial surrogate code, which is used to distribute the total county emissions into the appropriate model grid cells. The surrogate codes represent the column of county fraction data in the spatial allocation file.   This is accomplished with a header record in the gridded surrogate data file that indicates the 'name', or code, to be used for each column.

> ➢ **Special Note**
> In previous versions of GRDEM the surrogate code was an integer value
> which represented the column of fractional data in the gridded surrogate
> file. Surrogate code "1" represented the first column of fractional data, code
> "5", the fifth column.
>
> In the current release the surrogate code is a 3-character field that allows
> the user to assign an acronym to the data **column** which is easier to
> remember and QA. Any existing surrogate cross reference files and
> gridded surrogate data files can still be used in GRDEM. The numeric code
> is simply treated as a character code.

Surrogate codes may represent distribution by area, population, land use type, roadway, airport, railroad, etc. This file utilizes the best match criteria described in Section 2.4; accordingly, the user may specify spatial surrogate assignments by state and/or county by entering non-zero values in the FIPS field. For example, a state/county code of "00000" would mean that a SCC(ASC)/spatial surrogate assignment would apply for all counties within the modeling domain (unless more specific assignments for that state and/or county are included elsewhere in the cross-reference file); "*nn*000" would apply to all counties in state *nn*; and "*nnmmm*" would apply only to county *mmm* in state *nn*.   Any record that contains the character "#" in column 1 will be skipped. This allows imbedded comments and notes to be included in the file.

Exhibits 3-63 and 3-64 show examples of the different types of gridded surrogates cross reference files.

Table 3-40. SCC(ASC)/spatial allocation surrogate code cross-reference file input into the GRDEM module. This is for when the secondary surrogate codes are used.

Line	Variable	Columns	Type	Description

1+	FIPXRF	1-5	C	FIPS code of state/county:
				  00000 = applies to all counties in region
				  *nn*000 = applies to all counties in state *nn*
				  nnmmm = applies to county *mmm* in state *nn*

	SUBRGN	7-11	C	Subregion code
	ISGXRF(1)	13-15	C	Primary Surrogate code
	ISGXRF(2)	16-18	C	Secondary Surrogate code
	ISGXRF(3)	19-21	C	Tertiary Surrogate code
	SCCXRF	23-32	A	Area Source Category (ASC)
	LABEL	33	C	Source classification label (optional)

Table 3-41. SCC(ASC)/spatial allocation surrogate code cross-reference file input into the GRDEM module. This is for when only primary surrogate codes are used.

Line	Variable	Columns	Type	Description

1+	FIPXRF	1-5	C	FIPS code of state/county:
				  00000 = applies to all counties in region
				  nn000 = applies to all counties in state nn
				  nnmmm = applies to county mmm in state nn

	SUBRGN	7-11	C	Subregion code
	ISGXRF	13-15	C	Surrogate code
	SCCXRF	17-26	A	Area Source Category (ASC)
	LABEL	27-80	C	Source classification label (optional)

It is important to note that the file formats are different for the "secondary surrogates" and "only primary surrogate" files. You can <u>not</u> simply change the flag in the /GRDEM/ packet. You must also change the input file format.

```
# This is an example of secondary/tertiary surrogate codes
00000      INDTPPTCA 2102002000 Industrial Bituminous/Subbituminous Coa
00000      INDTPPTCA 2102004000 Industrial Distillate Oil

00000      INDTPPTCA 2102005000 Industrial Residual Oil

00000      INDTPPTCA 2102006000 Industrial Natural Gas

00000      INDTPPTCA 2102006001 Natural Gas All Boilers
   00      INDTPPTCA 2102007000 Industrial Liquified Petroleum Gas
# This is an imbedded comment line and will be skipped
  .
  .
```

Exhibit 3-63. Example of gridded surrogates cross reference file read by GRDEM. This is used when the secondary surrogates switch is turned on.

```
# This is an example of only primary surrogate codes
# Note the different file format from secondary/tertiary file
00000      IND   2102002000 Industrial Bituminous/Subbituminous Coa
00000      IND   2102004000 Industrial Distillate Oil
00000      IND   2102005000 Industrial Residual Oil
00000      IND   2102006000 Industrial Natural Gas
00000      IND   2102006001 Natural Gas All Boilers
00000      IND   2102007000 Industrial Liquified Petroleum Gas


  .
  .
  .
00000      RUR   2260001000 Recreational Vehicles
```

Exhibit 3-64. Example of gridded surrogates cross reference file read by GRDEM. This is used when the secondary surrogates switch is turned off.

The fourth input file contains information on the distribution of each type of surrogate on the CAMx modeling domain (Table 3-42). Each grid cell is identified by the geographical coordinates of the lower left corner of the cell and the UTM zone, if applicable. Essentially, all grid cells of the defined modeling domain will cover land area in one or more counties; accordingly, each gridded surrogate record must contain the state/county FIPs code. Optionally, a subregion code may be included for a more detailed assignment. The exception to this will be in a modeling domain which encompasses large portions of ocean water. Each of the surrogate fields on a record indicate the fraction of the county total for that surrogate contained in the grid cell. Total county emissions for each source category will be allocated to each grid cell based on the fraction of the assigned surrogate field calculated for the cell.

> ➢ **Special Note**
> In previous versions of GRDEM the surrogate code was an integer value which represented the column of fractional data in the spatial allocation surrogate file. Surrogate code "1" represented the first column of fractional data, code "5", the fifth column.
>
> In the current release the surrogate code is a 3-character field that allows the user to assign an acronym to the data **column** which is easier to remember and QA. Any existing surrogate cross reference files and spatial allocation surrogate data files can still be used in GRDEM. The numeric code is simply treated as a character code.

The first record of the spatial allocation surrogate file represents the area of coverage of the data in the file. The second record, a recent enhancement to the spatial allocation surrogate file, begins with the keyword 'CODES'. This allows the user to assign code names to each surrogate column and is used to match the cross reference field to a surrogate code. The order in which the surrogate codes occur on the record represent the order of the surrogate data. Exhibit 3-65 shows an example of the spatial allocation surrogate file. In this example the first surrogate column is assigned surrogate code 'TCA', total county area, the second is assigned surrogate code 'TPP', total population, etc. This code, together with the surrogate code listed in the cross reference file, is used to identify which column of data to use for each source category.

An additional enhancement to the spatial allocation file is that any record that contains the '#' character in column 1 will be skipped, allowing the user to document the development of the spatial allocation file in detail.

Table 3-42. Gridded spatial allocation surrogate file input into the GRDEM module.

	Variable	Columns	Type	Description
1	BUTME	1-10	R	Minimum X direction coordinate
	BUTMN	11-20	R	Minimum Y direction coordinate
	EUTME	21-30	R	Maximum X direction coordinate
	EUTMN	31-40	R	Maximum Y direction coordinate
	IUZONE	41-50	I	UTM zone, if appropriate
	XCELSZ	51-60	R	X direction cell size
	YCELSZ	61-70	R	Y direction cell size
				Line 2 is optional. If the keyword CODES is not found the column number is assigned to the surrogate code.
2	KEYWORD	1-5	C	Keyword "CODES"
	CODNM()	42-191	C	3-character code names representing each column of surrogate data. These codes must match the codes assigned to state/county/SCC in the surrogate cross reference file.
3+	FIPSRG	1-5	C	FIPS code of state/county
	SUBRGN	7-11	C	Subregion code
	XCDSRG	12-21	R	X direction coordinate of lower left corner of grid cell
	YCDSRG	22-31	R	Y direction coordinate of lower left corner of grid cell
	IZNSRG	32-41	I	UTM zone, if appropriate
	SURGIN( )	42-191	R	Fraction of county totals in cell for each surrogate. The order in this list corresponds to the surrogate code. For example, the first fraction is surrogate 1, the second is surrogate 2, etc. Each value is in a field of 10 columns.

> **Important Note**
> The spatial allocation surrogate file **must be pre-sorted** by FIPS.
>
> In order to reduce processing time the sort is assumed to be done prior to GRDEM. This can easily be accomplished with a Linux 'sort' command.

ENVIRON

```
#  file developed 20 Aug 2008 at ENVIRON
#  columns/codes represent the following
#  TCA - total county area
#  TPP - total population
#  UPP - urban population
#  RPP - rural population
#  THU - urban housing
#  TRU - rural housing
#
   -252000  -1728000   1296000   -180000         0 12000.000 12000.000
# the surrogate codes are specified here
CODES                                         TCA      TPP      UPP      RPP      THU      TRU
#  spatial allocation data starts here
01001       1200000.0 -720000.0       0  0.010609 0.031712 0.000000 0.050727 0.033086 0.0000
01001       1200000.0 -708000.0       0  0.025946 0.089234 0.000000 0.142743 0.097310 0.0000
01001       1212000.0 -744000.0       0  0.007318 0.000431 0.000000 0.000690 0.000482 0.0000
01001       1212000.0 -732000.0       0  0.046129 0.107611 0.000000 0.172139 0.109099 0.0000
01001       1212000.0 -720000.0       0  0.091955 0.093768 0.000000 0.149995 0.097105 0.0000
01001       1212000.0 -708000.0       0  0.078770 0.006486 0.000000 0.010375 0.006386 0.0000
01001       1224000.0 -744000.0       0  0.001886 0.000111 0.000000 0.000178 0.000124 0.0000
01001       1224000.0 -732000.0       0  0.059059 0.003711 0.000000 0.005937 0.004105 0.0000
01001       1224000.0 -720000.0       0  0.093876 0.015149 0.000000 0.024232 0.015040 0.0000
01001       1224000.0 -708000.0       0  0.093452 0.016113 0.000000 0.025774 0.015584 0.0000
01001       1224000.0 -696000.0       0  0.038873 0.006954 0.000000 0.011124 0.006645 0.0000
01001       1236000.0 -732000.0       0  0.046042 0.006843 0.000369 0.010726 0.006894 0.0000
01001       1236000.0 -720000.0       0  0.093871 0.027776 0.007033 0.040215 0.026804 0.0000
```

Exhibit 3-65. Example of spatial allocation surrogate file read by GRDEM.

The fifth input file, which is optional, contains definitions of transportation links for those categories for which such data is available (commonly, onroad motor vehicles, railroad locomotives, aircraft landings and takeoffs, and shipping vessels) (Table 3-43). GRDEM assigns emissions from these sources only to those cells in the region containing a portion of length of specified link type. Links must have a length greater than zero; they can be contained entirely within a single cell, or may span several cells. If the SCC(ASC) spatial surrogate cross-reference file specifies a particular link data type to be used to spatially allocate emission from a grid source category and the link definition file does not contain data for that link type for the indicated county, the emissions record is not processed and written to the error file in EMAR format.

Table 3-43. Link definition data file input into the GRDEM module.

Line	Variable	Columns	Type	Description
1+	FIPLNK	1-5	C	FIPS code of state/county
	CTYPE	6-10	C	Link type: '101' = Limited access roadways '102' = Railroad '103' = Airports '104' = Shipping '105' = Disposal sites
	XCDBEG	11-20	R	X direction coordinate of beginning of link
	YCDBEG	21-30	R	Y direction coordinate of beginning of link
	XCDEND	31-40	R	X direction coordinate of end of link
	YCDEND	41-50	R	Y direction coordinate of end of link
	IZNLNK	51-60	I	UTM zone, if appropriate

Output Files

GRDEM produces 5 output files: a message file, the CAMx surface emissions file or the gridded EMBR, an optional (and obsolete) county/ASC emissions totals file, an EMAR error file containing any input records that GRDEM was unable to process, and an optional gridded surrogate report.

The first section of the message file lists input and output file names and region definition parameters, followed by a summary of the number of grid cells encompassed by each county and the grid cells crossed by each link (if link data are utilized). The next section summarizes input and output emissions totals by criteria pollutant for the entire modeling domain. The totals include elevated source emissions totals and total emissions for records that were either skipped or written to the EMAR output file. This section may be followed by a series of warning messages indicating the counties specified in the /COUNTY/ packet of USERIN for which no EMBR records were encountered. The final section of the GRDEM message file contains tables of emissions totals as specified in the /CRITERIA TABLES/ and /SPECIES TABLES/ packets of the USERIN file. Exhibit 3-66 shows an example of a GRDEM message file.

```
              EPS3 GRDEM module v. 1.00 Aug 2004      07/25/07 18:43:47

          Input Files
        USERIN file                    :../inputs/userin.test_problem.wkd
        Input EMBR file                :../embr/embr.tmprl.ar.test_problem.wkd
        Surg. XREF file                :../inputs/spatial.allocation.xref.Aug03
        Gridded Surg. file             :../inputs/gridded.surrogates.TX.12km
        No link definition data provided.

          Output Files
        Emissions file                 :../emiss/emiss.ar.test_problem.wkd
        ASC/FIPS Emiss file            : Not requested.
        ERROR file                     :../error/emar.grdem.ar.test_problem.wkd
        Surrogate Report file          : Not requested.

              EPS3 GRDEM module v. 2.01 Jun 2008      07/25/08 18:43:47

        File note                      :CAMx Modeling of Tx regional, 9/13/99
        Episode date (Calander)        :990913
        Episode date (Julian)          :99256
        Beginning hour                 :    0
        Ending hour                    :   24
        Grid origin (km)               : (  -108.000,  -1584.000)
        UTM zone                       :    0
        Grid cell width (km)           : (    12.000,    12.000)
        Number of cells                : (  135,  138)
        Number of counties             :  213
        Output is UAM                  :YES

        Number of ASC-SCC/surrogate XREF records read:      466


        Number of grid cells in county 48001     :     32
        Number of grid cells in county 48005     :     28
.
            .
            .
        Number of grid cells in county 48507     :     30


            Total Emissions Processed
                English Tons


                      NOX       VOC       CO        SO2
        -------------------------------------------------------------------
        Input Emissions      444.0641   290.3760   2887.0341      0.
        Output Emissions     379.1137   265.1964   2653.5143      0.
        Elevated Emissions      0.         0.          0.         0.
        Mapped to Sec Surg    11.5134    10.8279    206.5085      0.
        Mapped to Tert Surg    0.1867     0.0769      2.1050      0.
        Written to EMAR         0.         0.          0.         0.
        Emissions Skipped     24.3421    12.0327     92.7044      0.
        -------------------------------------------------------------------
```

Exhibit 3-66. Example of a GRDEM message file.

The emissions output file created by GRDEM contains a gridded inventory of surface emissions either in CAMx-ready format or EMBR format (Table 2-14). The EMBR formatted file can be further processed by other EPS3 modules, while the model-ready emissions file may be merged with other CAMx surface emissions files using the MRGUAM module.

The county/ASC output file is an obsolete file and should be left blank in the GRDEM job script. The next output file, which may be empty, contains the emission records (in EMAR format) that GRDEM could not process. The most likely cause for records to be written to this file is that the SCC(ASC) code on the record was cross-referenced to a surrogate code for which no spatial allocation surrogate data were provided for that county.

The final output file, an optional report, allows detailed review of the spatial allocation process. (Exhibit 3-67) This report, depending on the number of counties and SCCs in the inventory, may be quite large. It provides criteria pollutant input and output totals by state/county code, SCC, the assigned surrogate code, and a flag indicating if the code was a primary ('P'), secondary ('S') or tertiary ('T') mapping. The surrogate report increases the processing time of the GRDEM module, as such, it should not necessarily be included in every job script. It should be reviewed when a new spatial allocation file has been developed or when a new emissions inventory is processed. The report can be imported into a spreadsheet for quick subtotals. Optionally a quick Unix 'grep' to extract records of interest could also be preformed to reduce the number of records to review. One could extract a single county of concern or all non-primary surrogates for detailed review.

> ➤ **Special Note**
> It is only necessary to change an existing GRDEM job script if the optional output gridded surrogate report is being requested. If the additional filename is not provided GRDEM assumes that the report has not been requested.

Exhibit 3-68 shows an example of a GRDEM job script.

```
                    Criteria Pollutant Emissions by FIPS, SCC, Surrogate Code, and Surrogate Flag
                                              English Tons/Day


   FIPS  SCC        Srg Flg      Input       Output      Input       Output      Input       Output
                                 NOX         NOX         VOC         VOC         CO          CO
   --------------------------------------------------------------------------------------------------
   48001 2260001010 21  P        0.0002      0.0002      0.0560      0.0560      0.0437      0.0437
   48001 2260001030 21  P        0.0002      0.0002      0.0703      0.0703      0.0543      0.0543
   48001 2260001060 2   S        0.0003      0.0003      0.0016      0.0016      0.0339      0.0339
   48001 2260002006 6   T     0.398E-04      0.          0.0022      0.          0.0055      0.
   48001 2260002009 6   T     0.121E-05      0.       0.616E-04      0.          0.0002      0.
   48001 2260002021 6   T     0.121E-05      0.       0.688E-04      0.          0.0002      0.
   48001 2260002027 6   T        0.          0.          0.          0.       0.121E-05      0.
   48001 2260002039 6   T     0.857E-04      0.          0.0044      0.          0.0135      0.
   48001 2260002054 6   T        0.          0.       0.966E-05      0.       0.434E-04      0.
   48001 2260003030 2   S        0.          0.       0.574E-05   0.574E-05   0.275E-04   0.275E-04
   48001 2260003040 2   S        0.          0.          0.          0.       0.230E-05   0.230E-05
   48001 2260004015 2   S     0.394E-05   0.394E-05      0.0006      0.0006      0.0010      0.0010
   48001 2260004016 2   S     0.157E-04   0.157E-04      0.0015      0.0015      0.0034      0.0034
   48001 2260004020 2   S     0.434E-04   0.434E-04      0.0049      0.0049      0.0096      0.0096
   48001 2260004021 2   S        0.0003      0.0003      0.0152      0.0152      0.0457      0.0457
   48001 2260004025 2   S     0.852E-04   0.852E-04      0.0104      0.0104      0.0181      0.0181
   48001 2260004026 2   S     0.985E-04   0.985E-04      0.0054      0.0054      0.0156      0.0156
   48001 2260004030 2   S     0.536E-04   0.536E-04      0.0075      0.0075      0.0117      0.0117
   48001 2260004031 2   S        0.0002      0.0002      0.0121      0.0121      0.0335      0.0335
```

Exhibit 3-67. Example of the optional gridded surrogate report.

```
#!/bin/csh
#
#   --- Sample job script for running the
#       EPS3 module GRDEM
#
set EXEC = /models/eps3/src
#
set SCENARIO = test_problem
#
foreach DAY (wkd sat sun)
#
#rm -f ../msg/msg.grdem.ar.$SCENARIO.$DAY
rm -f ../emiss/emiss.ar.$SCENARIO.$DAY
rm -f ../error/emar.grdem.ar.$SCENARIO.$DAY
#
echo "---------------------------------------------------"
echo "     Running GRDEM for $SCENARIO - area sources"
echo "          Day - $DAY"
echo "---------------------------------------------------"

$EXEC/grdem/grdem << IEOF
USERIN file         :../inputs/userin.$SCENARIO.$DAY
Input EMBR file     :../embr/embr.tmprl.ar.$SCENARIO.$DAY
Surg. XREF file     :../inputs/spatial.allocation.xref.Aug03
Gridded Surg. file  :../inputs/gridded.surrogates.TX.12km
Links data          :
Output Messages     :../msg/msg.grdem.ar.$SCENARIO.$DAY
Output Emissions    :../emiss/emiss.ar.$SCENARIO.$DAY
Output ASC/FIPS Ems:
EMAR error file     :../error/emar.grdem.ar.$SCENARIO.$DAY
Surg report         :
IEOF
end
```

Exhibit 3-68. Example of a GRDEM job script.

3.15   MRGUAM

Different source types of emissions data (e.g., point, area, mobile, biogenic) can be processed separately through EPS3 to facilitate both control strategy analysis and quality control tracking. Consequently, the EPS3 core system includes a module for merging multiple emissions files into one file for modeling. The MRGUAM (**MeRG**e **UAM** files) module will

   Combine the low-level emissions data from virtually any number of CAMx-format files into a single file, and

   Apply domain-wide, across-the-board multiplicative factors by chemical mechanism compound for any (or all) of the input emissions files.

This second function creates emissions inventories for use in "control sensitivity" applications of CAMx. This type of CAMx application is designed to estimate the overall amount of emissions reductions required to produce a desired change in pollutant concentrations. Control sensitivity applications should not be confused with control strategy applications, which attempt to simulate as accurately as possible the effects of a specific set of control measures applied at the individual source level.

Although different emissions files used in the same CAMx application must all be appropriate to the region and time period being modeled, they may contain different chemical mechanism compounds. Most CAMx surface emissions files will have been created by the GRDEM module, with the notable exception of the biogenic emissions file (which may be created outside of the EPS3 system). MRGUAM will accept as input any CAMx-ready surface emissions file, regardless of its origin. It sums the emissions from all of the input emissions files, by hour, grid cell, and chemical mechanism compounds, and writes the sum to a single file.

Input Files

MRGUAM reads the USERIN file and one or more surface emissions files, depending on the intended use of the module.

MRGUAM reads three packets from USERIN:

/SPECIES LIST/ MRGUAM reads this packet of the user input file (Table 2-11) in order to obtain the species list. The species list used for the output merged file is contained in this packet. Only species listed in this packet will be included in the merged output file. This allows the user to create an emissions file that excludes a species present in one or all of the input files.

/DATE/   This packet (Table 2-6) contains the episode definition which MRGUAM uses to determine the header information for the output emissions file.

/REGION/   MRGUAM reads this packet (Table 2-7) to determine the size and configuration of the modeling domain grid.

MRGUAM can read any number of CAMx-ready surface emissions files. If the user is running MRGUAM only to apply across-the-board factors to a file, only the one emissions file will be

required. Like the other modules that accept multiple EMBR input files, MRGUAM reads the names of the input EMBR files from the standard input file, i.e., the job script used to execute the module. See Exhibit 3-69 for an example. The keyword "END" must immediately follow the list of input file names in the command file to signal MRGUAM that all input files have been read.

Emission adjustment factors for each input emission file are also read from the standard input file. The name of the chemical mechanism compound (10-characters) and the adjustment factor (format f10) are input on the lines following the emission file name. Only those compounds to be adjusted need be specified. MRGUAM verifies that the controlled compound is included in the /SPECIES LIST/ packet.

Output Files

In addition to the merged CAMx emissions file, MRGUAM creates a message file containing tabular emissions totals. The first section summarizes input and output file names, followed by tables of hourly emissions totals by chemical mechanism compounds for each input file and for the output merged file. The final table in the message file contains the emissions totals summed over all hours for each input file and the merged output file. The totals for the input emissions files reflect the application of any multiplicative factors specified by the user in the standard input file. Emissions totals are generated only for the chemical mechanism compounds used for the output emissions file.

Exhibit 3-69 shows an example of a MRGUAM job script.

```
#!/bin/csh
#
#    --- Sample job script for running the
#        EPS3 module MRGUAM
#
set EXEC = /models/eps3/src
#
set SCENARIO = test_problem
#
foreach DAY (wkd sat sun)
#
rm -f ../msg/msg.mrguam.$SCENARIO.$DAY
rm -f ../emiss/emiss.$SCENARIO.$DAY
#
echo "---------------------------------------------------"
echo "    Running MRGUAM for $SCENARIO"
echo "        Day - $DAY"
echo "---------------------------------------------------"

$EXEC/mrguam/mrguam << IEOF
USERIN file        :../inputs/userin.$SCENARIO.$DAY
FILE 1             :../emiss/emiss.ar.$SCENARIO.$DAY
                   :OLE        0.8
                   :PAR        0.8
                   :TOL        0.8
                   :XYL        0.8
                   :FORM       0.8
                   :ALD2       0.8
                   :ETH        0.8
                   :MEOH       0.8
                   :ETOH       0.8
                   :ISOP       0.8
FILE 2             :../emiss/emiss.pts.$SCENARIO.$DAY
                   :NO         0.5
                   :NO2        0.5
FILE 2             :../emiss/emiss.bio.$SCENARIO.$DAY
                   :/END/
Output Messages    :../msg/msg.mrguam.$SCENARIO.$DAY
Merged emiss file  :../emiss/emiss.$SCENARIO.$DAY
IEOF
end
```

Exhibit 3-69. Example of a MRGUAM job script.

4. UTILITY DESCRIPTIONS

As discussed in Section 2.2, the EPS3 system includes utility programs to assist the user in creating some of the required input files and generating reports for quality control. This section describes the EPS3 utilities:

Input Preparation Utilities

    EMSCVT (chemical mechanism split factors and SCC(ASC)/speciation profiles cross reference file)

    TMPFAC (temporal profiles and SCC(ASC)/temporal profiles cross reference file)

EMBR Reporting Utility

    EMBRET (conversion from EMBR to EMAR; retrieval of selected EMBR records)

Output Reporting Utility

    SPLTEM (hourly, gridded, speciated emissions; for individual species e.g. propylene)

4.1 EMSCVT

The EMSCVT (**EM**i**S**sions **C**on**V**er**T** factors) utility creates two files: (1) factors used to disaggregate (or "split") criteria pollutant emissions into air-quality model (AQM) species and (2) the SCC(ASC)/speciation profiles cross-reference file required by the CHMSPL module. CHMSPL, details in Section 3.5, performs the conversion of criteria pollutant emissions into AQM species and creates a chemically speciated EMBR file. The split factors file consists of multiplicative factors for converting grams of criteria pollutant emissions into moles of chemical mechanism compound for each speciation profile. The SCC(ASC)/speciation profiles cross-reference file contains the speciation profile code assignments for each SCC(ASC) code; it may also contain source-specific speciation profile assignments. The user has the option of either generating completely new versions of these files or of updating existing versions of one or both of these files. EMSCVT calculates the split factors for each speciation profile based on the weight fractions of individual chemical compounds associated with that profile and the mechanism mapping for each compound. The mechanism mapping determines how much of the mass of that compound is attributed to each chemical mechanism compound.

Terminology

- **Chemical compounds** are real compounds, e.g., butane, toluene
- **Speciation profiles** define emissions composition as weight fraction of real compounds. The sum of the weight fractions should be 1.
- **AQM species** are chemical species used in chemical mechanisms, e.g., Carbon Bond species PAR, TOL and SAPRC species ALK3, ARO1
- **Mechanism mapping** is the unique matrix of assignments from chemical compounds to AQM species
- **Split-factors** define emissions composition as moles of AQM species per gram of emissions

---

EMSCVT allows the user to specify which AQM species will be included in the split factors file. EPS3 supports up to 24 AQM species by default and the number of AQM species can be increased by changing the MXSPEC parameter and recompiling the source code.

For most modeling applications the user will not need to execute EMSCVT; the split factors file and SCC(ASC)/speciation profiles cross-reference file provided with the EPS3 distribution may be used for chemical speciation of emissions. The default files are based on EPA's SPECIATE 4.0 VOC speciation profiles (the EPA speciation profiles are the preferred source of speciation data in the absence of source-specific speciated emissions). The primary reasons that users might employ the EMSCVT utility are (1) to create source-specific speciation profiles, (2) to modify existing speciation profiles for a particular control scenario (e.g., use of reformulated gasolines in light-duty automobiles) and (3) control a specific molecular compound, for example, benzene.

Calculating Split Factors

In the following discussion, "chemical compound" refers to a specific chemical (e.g., carbon tetrachloride, benzene, or 1,3-butadiene) and AQM species is a chemical species used in air quality models (e.g., Carbon Bond species PAR, TOL).

The profile weights file defines speciation profiles by identifying the chemical compounds that contribute to the total mass of emissions and their corresponding weight fractions. Chemical compounds are identified by 5-digit AIRS pollutant code; weight fractions are defined as the ratio of the mass of emissions for that chemical compound to total mass emissions. By definition, the sum of the weight fractions for a profile should equal one. The profile weights file optionally contains source identification codes for which the profile is applicable (FIPS state/county, plant identification, stack identification, and SCC(ASC) codes), this allows definition of source specific speciation profiles.

> ➢ **Updating Inputs**
>
> To use EMSCVT to modify the split factors or cross reference for an existing profile code, it is only necessary to supply data for the profiles to be updated. Along with the updated profiles, supply the default split factors file and cross reference file as input to EMSCVT. Only those records in these files for the updated profile codes will be affected; records for all other speciation profiles will correspond to those in the original input files.

For each speciation profile, EMSCVT computes the split factor for each AQM species based on (1) the weight fractions of chemical compounds in the profile (from the weight profiles input file), and (2) the mechanism mapping for each compound (specified in the compound data base input file). Compound data base files are supplied with the EPS3 distribution for the CB4, CB05 and SAPRC-99 chemical mechanisms. The compound data base files include an extensive library of compounds and it is a rare situation when there is a need to update or modify the compound data base. The mechanism mappings are specified in units of molecules of AQM species per molecule of chemical compound. The sum of mechanism mapping factors for a specific chemical compound will not necessarily equal one. For each speciation profile included

in the input profile weights file, EMSCVT computes the total split factor for each AQM species by multiplying the mechanism mapping for each compound by the weight fraction of that compound and summing the AQM species contributions for the profile.

Because emissions inventories can report the mass of organic compounds differently (for example as VOC or TOG), EMSCVT must account for how the input hydrocarbon emissions are reported. Similarly, air quality modeling emission inventories can be prepared as VOC or TOG and EMSCVT provides the option of selecting whether split factors will be calculated as VOC or TOG. You should select the EMSCVT VOC/TOG options based on (1) the type of data included in the initial inventory (AFS and AMS) work files, and (2) the compounds you wish to include in the speciated emissions file. Table 4-1 shows the different combinations of VOC/TOG conversions supported by EMSCVT. Option 3 is the most likely option for current modeling applications in the United States.

Table 4-1. EMSCVT Emission type flags.

Option	EMSCVT User Input Flag	EMSCVT User Output Flag	Input Emissions Reported As	Split Factors Will Produce
1	VOC	VOC	VOC	VOC
2	TOG	VOC	TOG	VOC
3	VOC	TOG	VOC	TOG
4	TOG	TOG	TOG	TOG

Option 1: Input emissions are assumed to be VOC and the modeling inventory will be VOC. With this option, EMSCVT will remove any compound in the speciation profile that is considered a non-VOC (as specified by the VOC flag for each species in the compound data base according to EPA rules) and renormalize the profile before calculating split factors.

Option 2: Input emissions are assumed to be TOG and the modeling inventory will be VOC. With this option, EMSCVT will remove any compound in the speciation profile that is considered a non-VOC but will not renormalize the profile before calculating the split factors. Notice that this leads to a total weight for the profile that is less than one. Using a split factors file prepared with this option causes the CHMSPL module to effectively remove the non-VOC portion of the inventory during chemical speciation.

Option 3: Input emissions are assumed to be VOC and the modeling inventory will be TOG. With this option, EMSCVT will remove any compound in the speciation profile that is considered a non-VOC and renormalize the profile. However, before calculating the split factors EMSCVT will add the non-VOC compounds back into the profile. Notice that this leads to a total weight for the profile that exceeds one. When using split factors produced using this option the total emissions will likely increase after processing through the CHMSPL module. The CHMSPL module will effectively add the non-VOC portion back into the inventory before performing the speciation.

Option 4: Input emissions are assumed to be TOG and the modeling inventory will be TOG. With this option, EMSCVT ignores the VOC flag in the compound database and processes each profile as is.

In addition to creating or updating the split factors file, EMSCVT gives the user the ability to

update or create the SCC(ASC)/speciation profiles cross-reference file used by the CHMSPL module. This feature is seldom used, as it is just as easy to update the default cross reference file manually. In previous versions of EPS, the cross reference file contained information that depended on the speciation weight profiles. That is no longer the case. It is recommended that any updates to the cross reference file be performed using a text editor.

Source-Specific Speciation Profiles

For some sources, local data may be available that describes the exact chemical makeup of the emissions generated by the source. To model a source using local data it is necessary to calculate split factors specific to the source, as opposed to using a general speciation profile. To create a source-specific speciation profile for use in EPS3:

1. Define a new 5-character speciation profile code to be assigned to the source.

2. Update the default SCC(ASC)/speciation profiles cross reference file by adding a record which maps the specified source to the newly created profile code. As much detail (county ID, plant ID, etc.) should be provided so the source can be uniquely identified.

3. Create a profile weights file containing the AIRS pollutant codes and weight fractions for all of the chemical compounds produced by the source.

4. Run the EMSCVT program.

5. Append the contents of the new split factors to the end of the default split factors file.

Source-Specific Speciation Profile Tip

User-assigned source-specific speciation profile codes should be defined as a complete 5-character string, using non-numeric characters if possible. Since all of the default speciation profile codes are 4-character strings using numbers only, adhering to this practice will ensure that new profile codes can be easily distinguished from the defaults. In addition, this convention prevents the user from inadvertently assigning an existing EPA profile code for a source-specific speciation profile, which would most likely result in incorrect chemical speciation for those sources referenced to the existing EPA speciation profile.

Input Files

The EMSCVT utility requires up to five input files: the EMSCVT user input file, the profile weights data file, the compound data base (mechanism mapping) file, the default SCC(ASC)/speciation profiles cross-reference file (optional and obsolete), and the default split factors file (also optional).

The EMSCVT user input file (Table 4-2) contains user-specified parameters and the list of AQM species to produce. The first parameter, the tolerance parameter, determines the range of values

EMSCVT will accept for a correct profile weight. The absolute value of one minus the sum of all weight fractions for a profile must be less than this value in order for the profile to be acceptable. If the tolerance parameter is exceeded, EMSCVT renormalizes the weight fractions. This option can be used to ensure that all weight profiles are complete. However, because of roundoff issues it is often difficult to get a profile that adds exactly to one. The tolerance value determines how much roundoff is acceptable. The second parameter indicates how the input emissions inventory is reported: as VOC or TOG. It is important that this parameter match the emissions inventory processed by EPS3, as a mismatch will cause emissions to be artificially increased or decreased during the speciation processing step. The third parameter specifies whether the split factors produced by EMSCVT will generate a VOC or TOG speciated inventory. The final section of the user input file contains the list of AQM species for which EMSCVT will compute split factors; for each species, the user must supply the species name, the criteria pollutant from which each AQM species is derived, the species molecular weight, and a default split factor to be used for that species (Exhibit 4-1). For AQM species included in the compound data base file, the user should specify a default split factor of 0.0. When using EMSCVT to update an existing split factors file (an optional input file), the species list from the existing file *must* correspond to the species list in the EMSCVT user input file.

Table 4-2. EMSCVT user input file.

Line	Variable	Columns	Type	Description
1		1-20		Not used
	EPSLON	21-30	R	Range used to determine a valid profile weight
2		1-20		Not used
	LVOCIN	21-100	C	Flag to specify input emissions types options are: VOC or TOG
3		1-20		Not used
	LVOCOUT	21-100	C	Flag to determine generated splits type: VOC = compute splits for VOC TOG = compute splits for TOG
4+		1-20		Not used
	SPCLST(*)	21-30	C	Air quality modeling compound name
	MOLWT(*)	32-36	C	Molecular weight for compound
	SPGRIT(*)	38-42	C	Criteria pollutant that creates this compound
	DEFSPL(*)	44-53	R	Default splits value for this compound

```
Valid weight range : 0.05
Input inventory is : VOC
Output splits for  : TOG
                   :OLE         32.0 VOC         0.0
                   :PAR         16.0 VOC         0.0
                   :TOL        112.0 VOC         0.0
                   :XYL        128.0 VOC         0.0
                   :FORM        16.0 VOC         0.0
                   :ALD2        32.0 VOC         0.0
                   :ETH         32.0 VOC         0.0
                   :MEOH        16.0 VOC         0.0
                   :ETOH        32.0 VOC         0.0
                   :ISOP        80.0 VOC         0.0
                   :NR          16.0 VOC         0.0
                   :NASN         1.0 VOC         0.0
```

Exhibit 4-1. User input file for EMSCVT.

The second input file for the EMSCVT utility, the profile weights file (Table 4-3), contains two types of information for profile codes. The first record type is optional. It supports a source specific speciation profile definition. If present, this record contains the source identification codes for which the profile applies: state/county FIPS, AFS plant identification code, AFS stack identification code, AFS point identification code, and SCC(ASC) code. The source identification fields are followed by the speciation profile code. The next series of records for each profile code contains the AIRS pollutant code and weight fractions for each chemical compound associated with the profile. An example profile weights file (with a single profile numbered 0000) is shown in Exhibit 4-2. Profile weights for each profile code must be grouped sequentially in the file.

Table 4-3. Profile weights file input to the EMSCVT utility.

Line	Variable	Columns	Type	Description
(Optional records)				
For each profile, provide list of SCC(ASC)/speciation profile cross-reference records to be updated in the input cross reference file.				
1	FIPXRF	1-5	C	FIPS code of state/county: 00000 = applies to all counties *nn*000 = applies to all counties in state *nn* *nnmmm* = applies county *mmm* in state *nn*
	FACXRF	7-16	C	Plant identification code from AFS (blank = applies to all facilities)
	ISTXRF	18-27	I	Stack identification code from AFS (blank = applies to all stacks)
	SCCXRF	29-38	C	Source classification code (SCC-ASC)
	PRFXRF	40-44	C	Profile code
(Mandatory records)				
For each profile to be updated, provide updated weight fractions.				
Line 2 is repeated for each chemical compound in weight profile.				
2+	PROFWT	1-5	C	Profile code
	ICMPCD	7-11	I	Pollutant code of chemical compound
	WTFRAC(*)	13-22	R	Weight fraction of chemical compound

```
0000  43105   0.1256
0000  43106   0.0581
0000  43107   0.0349
0000  43108   0.0442
0000  43109   0.0930
0000  43110   0.0116
0000  43111   0.1070
0000  43118   0.1488
0000  43119   0.0837
0000  43120   0.0116
0000  43121   0.0116
0000  43122   0.2581
0000  43125   0.0070
0000  43126   0.0023
0000  43127   0.0023
```

Exhibit 4-2. Example profile weights file input to EMSCVT.

The third EMSCVT input file, the compound data base (Table 4-4), contains the mechanism mapping that EMSCVT requires to create the composite split factors profile for each speciation profile code. The first record of this file indicates the number of AQM species for which mechanism mappings are specified; this record is followed by the list of chemical mechanism compound names. The remaining records specify chemical compound-specific data; the first field in each record contains the AIRS pollutant code for the chemical compound, followed by a 20-character field for naming the compound (not required, it is for notation) and the mechanism mapping for each specified chemical mechanism compound (Exhibit 4-3). The next field of each compound-specific record contains a flag indicating whether the compound is considered photochemically reactive ("VOC" designates a reactive compound, "TOG" indicates that the compound is a non-reactive molecular compound.) The final two fields contain the molecular weight of the chemical compound (required to accurately convert mass emissions to moles) and a flag indicating whether the compound is a toxic substance ("TOX" corresponds to toxic; blank indicates non-toxic).

Table 4-4. Compound data base file input to the EMSCVT utility.

Line	Variable	Columns	Type	Description
1	NSPCMP	1-10	I	Number of AQM species
2+	SPCCMP	1-10	C	Compound name; same order as fractions on records 3+
3+	ISAROD	1-5	I	AIRS pollutant code of compound
	CHMNAM	6-25	C	Chemical name of compound (not used)
	BNDFRC	27 - * end	R	Fraction for compound 1
	. . .			Fraction for compound NSPCMP
	LREACT	* end +2 - +5	C	Flag that determines if compound is considered reactive: VOC = reactive compound TOG = non-reactive organic compound
	MOLCMP	* end +6 - * end +15	C	Molecular weight of compound
	LTOXIC	* end +16	A	Flag for toxic substance TOX = toxic Blank = non-toxic

```
16
NASN       1.0
PAR        16.0
OLE        32.0
TOL        112.0
XYL        128.0
FORM       16.0
ALD2       32.0
ETH        32.0
ISOP       80.0
MEOH       16.0
ETOH       32.0
ETHA       32.0
IOLE       64.0
ALDX       32.0
TERP       160.0
NR         16.0
10001    cb4 olefin bond  1.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 VOC    1.00   cb4 olefin
...
43105 isomers of hexane  0.00 5.83 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.17 VOC   86.18   isomers
43106 isomers of heptan  0.00 6.81 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.19 VOC  100.21   isomers
43118    mineral spirits 0.00 6.34 0.00 0.06 0.09 0.00 0.00 0.00 0.00 0.01 0.06 0.00 0.01 0.00 0.00 0.04 VOC  110.10   mineral
43120 isomers of butene  0.00 1.00 0.50 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.50 0.00 0.00 0.00 VOC   56.11   isomers
...
45232 diphenyl ethane {  0.00 0.00 0.00 2.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 VOC  182.27   diphenyl
45233 ethyl-phenyl-phen  0.00 1.00 0.00 1.00 1.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 VOC  210.32   ethyl
45235      n-butylbenzene 0.00 3.00 0.00 1.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 VOC  134.22   n-butyl
45236 diisopropyl benze  0.00 4.00 0.00 0.00 1.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 VOC  162.28   diisoprop
...
86064   Diethyl Sulfate  0.00 4.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 VOC  154.19   Diethyl
90001        1-Dodecene   0.0010.00 1.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 VOC  168.32   1-Dodecene
90002 "2,3,5-trimethylh   0.00 9.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 VOC  128.26   "2,3,5
90023       methylbutene  0.00 3.33 0.33 0.00 0.00 0.33 0.33 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 VOC   70.14   methyl
90025       methylpentenes 0.00 3.50 0.50 0.00 0.00 0.00 0.25 0.00 0.00 0.00 0.00 0.00 0.25 0.00 0.00 0.00 VOC   84.16   methyl
```

Exhibit 4-3. Example of a portion of the CB05 compound database file input to EMSCVT.

The EMSCVT utility also has two optional input files: the default SCC(ASC)/speciation profiles cross reference file, and the default split factors file (Tables 3-19 and 3-20, respectively). If used, these files provide pre-computed data to be included in the output files created by EMSCVT. If the user does not specify these files, or if the specified files contain no data, the EMSCVT output files will only contain newly computed data.

Output Files

The EMSCVT utility produces three output files. The first of these, the EMSCVT message file (Exhibit 4-4), summarizes input and output filenames and information about the numbers of profiles computed and new records written. The message file also includes any warning or error messages generated during execution.

```
            EPS3 EMSCVT utility v. 1.2 Jun 2007       07/26/07 12:20:54


         Input Files
    User input file                :../inputs/emscvtin.udt.cb4.TOG_to_TOG
    Weight profiles file           :../inputs/emscvt.std_profiles.eps3
    Compound data base             :../inputs/cmpnd.db/cb4/TOG.07Jun14
    No input xref file.
    No splitting factors file.
    No control factors file.


         Output Files
    Output xref file               :
    Output splitting factors       :../outpts/spltfc.TOG/to/TOG/std/prf.cb4.07Jun14



             EPS3 EMSCVT utility v. 1.2 Jun 2007       07/26/07 12:20:54


    Range for valid profile      :/  0.9500,  1.0500/
    Input emissions should beTOG
    Output emissions will beTOG



    Species name        Molecular wt.          Criteria        Default split
    -------------------------------------------------------------------------
      OLE                 32.00                 VOC             0.0000E+00
      PAR                 16.00                 VOC             0.0000E+00
      TOL                112.00                 VOC             0.0000E+00
      XYL                128.00                 VOC             0.0000E+00
      FORM                16.00                 VOC             0.0000E+00
      ALD2                32.00                 VOC             0.0000E+00
      ETH                 32.00                 VOC             0.0000E+00
      MEOH                16.00                 VOC             0.0000E+00
```

Exhibit 4-4. Example of an EMSCVT output file.

The second EMSCVT output file is the new (or updated) SCC(ASC)/speciation profiles cross reference file to be used by the CHMSPL module. This file contains the speciation profile code assignments for each SCC(ASC) and any source identification codes specific to the profile.

The third output by the EMSCVT utility, the updated split factors file (Table 3-20), contains the newly calculated split factors for each speciation profile as well as any unmodified split factor profiles included in the original input split factors file, if an existing file was specified. The chemical mechanism compound order in the output split factors file corresponds to that of the default input file. Exhibit 4-5 provides a sample job stream for executing EMSCVT.

```
#!/bin/csh
#
#    --- Sample job script for running the
#        EPS3 module EMSCVT
#
#
set EXEC = /models/eps3/src
#
set SCENARIO = June14.2007
#
foreach mech (cb4 cb5 )
foreach f (VOC_to_VOC VOC_to_TOG TOG_to_VOC TOG_to_TOG)
#
echo "--------------------------------------------------"
echo "    Running EMSCVT for $SCENARIO "
echo "        $mech and $f"
echo "--------------------------------------------------"
#
rm -f ../msg/msg.emscvt.$f.std_profiles.$mech.eps3.$SCENARIO
rm -f ../outputs/splitfac.$f.std_profiles.$mech.eps3.$SCENARIO

$EXEC/emscvt/emscvt << IEOF
User Input file    :../inputs/emscvtin.udt.$mech.$f
Input Profiles     :../inputs/emscvt.std_profiles.eps3
Compound Database  :../inputs/compound.database.eps3.$mech.wTOG.$SCENARIO
Input XREF file    :
Input Split Factors:
Control Factors    :
Output Message file:../msg/msg.emscvt.$f.std_profiles.$mech.eps3.$SCENARIO
Output XREF file   :
Output Split Factor:../outputs/splitfac.$f.std_profiles.$mech.eps3.$SCENARIO
IEOF
end
end
```

Exhibit 4-5. Example of an EMSCVT job script.

4.2 TMPFAC

The TMPFAC (**TeMP**oral allocation **FAC**tor) utility creates and/or updates the temporal profiles file and the source/temporal profile cross reference file required as inputs to the EPS3 module TMPRL. This utility also allows the user to create source-specific temporal allocation profiles based on the throughput and operating schedule information contained in the AIRS AFS work file (Table 3-2).

The AIRS work file, which is the same file input to the PREPNT module, contains throughput and operating schedule information by state, county, plant, stack identification code, and SCC(ASC) codes. These data include seasonal throughput and information for hours per day, days per week, and hours per year. TMPFAC does not modify the AIRS work file in any way, but simply examines it to determine inventory-specific profiles.

TMPFAC reads the AIRS AFS work file, retrieving the throughput and operating schedule data for each record. TMPFAC then compares this information with the profiles in the existing temporal profiles file, processing the record in the following manner:

   (1) If the throughput and operating schedule data match existing profiles, and the assigned profile codes in the input SCC(ASC)/temporal profile cross reference files agree with the calculated profile, TMPFAC simply writes the existing temporal profile and cross reference records to the appropriate output files and retrieves the next AIRS record.

   (2) If the throughput and operating schedule data match existing profiles, but the source/temporal profile cross reference file contains different code assignments for that SCC(ASC), TMPFAC updates the cross reference file.

   (3) If the throughput and operating schedule data do not match existing profiles, and the cross-reference file does not contain a source-specific profile assignment for that source, TMPFAC updates both the temporal profiles file and the cross reference file.

   (4) If the throughput and operating schedule data do not match existing profiles, but the cross-reference file contains a source-specific profile assignment for that source, TMPFAC writes an error message to the message file and stops execution.

The seasonal throughput for a particular season is divided evenly among the months of the season. The seasons are defined as follows:

   Winter: January, February, and March
   Spring: April May, and June
   Summer: July, August, and September
   Autumn: October, November, and December

TMPFAC assigns weekly profiles for the AFS work file based on the data in the days/week field; diurnal profiles are assigned based on the hours/day field. If an AFS record contains valid data in the (optional) "start hour" field, TMPFAC will use the start hour and the number of hours/day in operation to calculate a diurnal profile. Again, TMPFAC will compare the calculated profiles with the existing profiles to determine any matches. If no match is found, a source-specific record is added to the temporal profiles file for that source.
TMPFAC assumes the following assignments regarding the operation schedule information

retrieved from the AIRS work files to determine the appropriate temporal profile codes for each source:

Days per week
      2 = Saturday and Sunday
      5 = Monday through Friday
      6 = Monday through Saturday
      7 = every day

Hours per day
       8 = hours 0900 through 1600 (9 a.m. to 5 p.m.)
      12 = hours 0700 through 1800 (7 a.m. to 7 p.m.)
      16 = hours 0800 through 2300 (8 a.m. to 12 a.m.)
      24 = every hour

If a record specifies number of days per week or hours per day other than those listed above (e.g., 1, 3, or 4 days per week or 6 hours per day), TMPFAC will assign the default temporal profiles for that source category.

Processing Note
The default temporal profiles and SCC(ASC)/temporal profiles cross reference files provided with EPS3 will generally suffice for most applications. However, the user should be aware that the data used to generate the default profiles and cross reference files were developed by the EPA based on general operating practices. Accordingly, the user should review the default profiles and assignments to ensure appropriateness for the particular modeling region.

The default profiles and cross-reference files provided with EPS3 can be input directly into the TMPRL core module; however, the user should use the TMPFAC utility to generate source-specific temporal distributions based on the information in the AFS file prior to executing TMPRL. If the throughput and operating schedule data fields of the AIRS work files contain only 'missing' data values, no modifications will be made to the temporal profiles and SCC(ASC)/temporal profiles cross reference files. Note that the TMPFAC utility may be run to modify the default files provided with EPS3, modify updated versions of these files, or generate completely new profiles.

Input Files

The TMPFAC utility reads three input files: a default SCC(ASC)/temporal profile cross-reference file (optional), a default temporal profiles file (optional), and the AIRS AFS work file. The default cross-reference and profiles files are provided with the EPS3 system.

The first input, the existing SCC(ASC)/temporal profile cross reference file (Exhibit 3-35; Table 3-26), contains state/county FIPS code, subregion code, plant ID code, and stack identification code. In the default file these fields contain "missing value" flags for every record ("00000" for FIPS, blank for subregion code, blank for plant ID and stack identification code). The rest of each record consists of an SCC code (for point sources), followed by the AIRS pollutant code

("00000" is the global code to specify all pollutants) and the monthly, weekly, and diurnal temporal profile codes assigned to that SCC. The SCC(ASC)/temporal profile cross reference file is an optional input. If this input is not specified then new cross reference records will be generated.

TMPFAC's second input is the existing temporal profiles file. If the user does not specify an existing temporal profiles file for input, the output temporal profiles file will consist entirely of source-specific profiles. The temporal profiles file contains four packets (Exhibit 3-36). The temporal profiles in all four packets are represented in the same manner; each time period (month, day of week, or hour) is assigned a weight that indicates the level of operation throughput or activity with respect to the other comparable time periods in the profile. The four packets are described below.

/MONTHLY/

    The /MONTHLY/ packet contains the temporal profiles that will be used by the TMPRL module to adjust annual or seasonal average emissions to episode month levels (Table 3-27). Each record in the /MONTHLY/ packet consists of a monthly temporal profile code followed by twelve temporal weight levels for the months of January through December. The final value on each record is the total of the weight levels for all 12 months.

/WEEKLY/

    The /WEEKLY/ packet consists of the temporal profiles used to adjust daily average emissions to account for variations in activity for different days of the week (Table 3-28). This packet is constructed analogously to the /MONTHLY/ packet; each record begins with the weekly temporal profile code, followed by the temporal weight levels for the seven days of the week. Note that the first weight level corresponds to Monday (not Sunday). Again, the final field on each record contains the total of the weight levels.

/DIURNAL WEEKDAY/

    This packet contains the temporal profiles that will be used to allocate daily emissions to each hour of the episode day for a weekday episode (i.e., Monday through Friday) (Table 3-29). Like the /WEEKLY/ and /MONTHLY/ packets, each record begins with a diurnal weekday profile code, lists the weight levels that will be used to distribute the emissions to the 24 hours of the day, and ends with the total of the weight levels for all hours. The first weight level corresponds to the hour from midnight to 1 a.m. (designated as hour "0000" in EPS3 and CAMx); the twenty-fourth weight level corresponds to the hour from 11 p.m. to midnight (hour "2300").

The third input file required by the TMPFAC utility is the AFS work file. Refer to Section 2.3 for a discussion of the AFS work file, and Table 3-2 for the file format definition.

Output Files

The TMPFAC utility produces three output files: a message file, an updated SCC(ASC)/temporal profile cross reference list, and an updated temporal profiles file. The TMPFAC message file (Exhibit 4-6) summarizes input and output file names, and number of records processed for each file. The message file will also contain any warning or error messages generated during execution (for example, warnings indicating that the global default profiles were assigned for a particular source).

```
      EPS3 TMPFAC utility v. 1.01 Oct 2004    07/26/07 12:26:07


          Input Files
 Input XREF file                :../../../inputs/temporal.allocation.xref_pts.
 Input profiles file            :../../../inputs/temporal.profiles.Aug03
 Input AFS file                 :../../../inputs/AFS.points.test_problem

          Output Files
 Output XREF file               :../outputs/temporal.n.xref_pts.test_problem
 Output profiles file           :../outputs/temporal.profiles.test_problem

 Number of temporal profile cross reference records read:      0
 Number of temporal profile cross reference entries:  2883
 Number of MONTHLY temporal profiles read:        26
 Number of WEEKLY temporal profiles read:        20
 Number of DIURNAL weekday temporal profiles read:        70
 Number of DIURNAL weekend temporal profiles read:        11

/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/

WARNING:  AFS file contains records with invalid days per week code.
          FIPS code: 48029
          Plant id : 0189
          Stack id : 1
          Point id : 089
          SCC code :   39999995
          Days/week code:     4
    Default values will be used for all such records.


/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/

   Number of AFS records processed:    23454
   Number of AFS records skipped:       17
   Number of cross reference entries added after AFS file:     2478
   Number of cross reference records written:     5361
   Number of /MONTHLY/          profiles written:      833
   Number of /WEEKLY/           profiles written:       20
   Number of /DIURNAL WEEKDAY/  profiles written:       93
   Number of /DIURNAL WEEKEND/  profiles written:       11
```

Exhibit 4-6. TMPFAC message file.

The second output file, the updated SCC(ASC)/temporal profile cross-reference file, is identical
in format to the original cross-reference file input to TMPFAC. Unlike the default file provided
with EPS3, however, the updated file may contain source-specific profile assignments. In other
words, TMPFAC may add records to this file which contain non-zero or non-blank data in the
state/county, plant, and stack identification code fields. When TMPRL is executed, the module
will use the source-specific profiles for those sources. If TMPFAC identifies no source specific
patterns, then the contents of the new cross-reference file will be identical to those of the original
file.

The final output file produced by the TMPFAC utility is the updated temporal profiles file, identical in format to the temporal profiles file input to the utility. Again, this output file will contain additional records corresponding to any source-specific profiles identified by TMPFAC from the AIRS AFS work file. If no source-specific profiles are created, the contents of this file will be identical to the input temporal profiles file. A sample job stream for TMPFAC is provided in Exhibit 4-7.

```
#!/bin/csh
#
#    --- Sample job script for running the
#        EPS3 module CHMSPL
#
set EXEC = /models/eps3/src
#
set SCENARIO = test_problem
#
rm -f ../msg/msg.tmpfac.$SCENARIO
rm -f ../outputs/temporal.allocation.xref_points.$SCENARIO
rm -f ../outputs/temporal.profiles.$SCENARIO
#
echo "------------------------------------------------"
echo "    Running TMPFAC for $SCENARIO "
echo "------------------------------------------------"
#
$EXEC/tmpfac/tmpfac << IEOF
Input XREF file    :../../../inputs/temporal.allocation.xref_points.Aug03
Input Profiles file:../../../inputs/temporal.profiles.Aug03
Input AFS          :../../../inputs/AFS.points.$SCENARIO
Output message     :../msg/msg.tmpfac.$SCENARIO
Output XREF file   :../outputs/temporal.allocation.xref_points.$SCENARIO
Output Profiles file:../outputs/temporal.profiles.$SCENARIO
IEOF
```

Exhibit 4-7. An example of a TMPFAC job script.

4.3 EMBRET

EPS3 utilizes an internal binary format for emissions files to reduce storage requirements and improve computation speed. In order for the user to readily examine, manipulate, or modify the emissions data, or to transfer data between computing platforms, the binary EMBR file must be converted to ASCII format.

The EMBRET (**EMBR RET**rieval and ASCII conversion) utility allows the user to convert an EMBR (binary) file to EMAR (ASCII) format. You may convert either all of the data in the EMBR file or a subset of the data. EMBRET reads each record of the EMBR file and checks the appropriate data fields to determine if the record meets the user's specifications for extraction. If the record meets the requirements, it is written in ASCII format to the output file.

Input Files

The EMBRET utility has two input files: an optional user input file and the EMBR file to be converted. The EMBRET user input file is used to specify which records of the EMBR file are to be extracted, converted, and written to the output EMAR file. If no input file name is specified, the entire EMBR file will be converted to EMAR format. The EMBRET user input file may contain any of the following packets, which may be specified in any order (Exhibit 4-8).

/COUNTY/   This packet (Table 4-5) contains a list of FIPS state/county codes for which to extract and convert records.

/PLANT/   This packet (Table 4-6) is used to make a list of facilities (using the facility identification code) for which to retrieve data.

/SCC/   This packet (Table 4-7) contains a list of Source Classification Codes and/or Area Source Category codes to extract.

/SIC/   This packet (Table 4-8) is used to make a list of Standard Industrial Codes for which to extract data.

/SUBGRID/   This packet (Table 4-9) specifies a rectangular subregion of the modeling domain for which to retrieve data; the packet is valid only if the EMBR data are gridded (i.e., contain valid I and J cell coordinates in the IJCELL field). This packet contains four parameters: the I (east-west) and J (north-south) grid cell coordinates for the lower left and upper right corners of the subregion. Note that grid cell coordinates are referenced according to the location of the upper right corner of the grid cell; for example, the grid cell located at the origin of the modeling grid is assigned I and J grid cell coordinates of (1, 1), not (0, 0).

> ➢ **Processing Note**
> The EMAR file produced by EMBRET can easily be loaded into a spreadsheet program or a database application. It is standard procedure to extract the entire EMBR file (by specifying a blank filename for the user input file) and post processing the output using another application. This provides the most flexibility in analyzing the data.

Table 4-5. /COUNTY/ packet of the EMBRET user input file.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	A	Packet identifier = /COUNTY/
2+		1-20		Not used
	CTYSCD(*)	21-25	A	FIPS state/county code
3	KEYEND	1-20	A	Packet terminator = /END/

Table 4-6. /PLANT/ packet of the EMBRET user input file.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	A	Packet identifier = /PLANT/
2+		1-20		Not used
	PLNTCD(*)	21-25	A	Plant code
3	KEYEND	1-20	A	Packet terminator = /END/

Table 4-7. /SCC/ packet of the EMBRET user input file.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	A	Packet identifier = /SCC/
2+		1-20		Not used
	RSCCCD(*)	21-30	A	Source Classification Code (SCC/ASC)
3	KEYEND	1-20	A	Packet terminator = /END/

Table 4-8. /SIC/ packet of the EMBRET user input file.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	A	Packet identifier = /SIC/
2+		1-20		Not used
	RSICCD(*)	21-24	A	Standard Industrial Classification Code
3	KEYEND	1-20	A	Packet terminator = /END/

Table 4-9. /SUBGRID/ packet of the EMBRET user input file.

Line	Variable	Columns	Type	Description
1	KEYWRD	1-20	A	Packet identifier = /SUBGRID/
2+		1-20		Not used
	IBEGTM	21-30	I	I-cell index of lower left corner of subregion
	JBEGTM	31-40	I	J-cell index of lower left corner of subregion
	IENUTM	41-50	I	I-cell index of upper right corner of subregion
	JENDTM	51-60	I	J-cell index of upper right corner of subregion
3	KEYEND	1-20	A	Packet terminator = /END/

```
/COUNTY/
Wilson, TX          :48493
/END/

/SIC/
Solvents Usage     :2401
/END/

/SCC/
Petroleum Transport :2505030120
/END/

/PLANT/
Texas Utilities    :0012
/END/

/SUBDRID/
Middle of domain    :       10        30        14        31
/END/
```

Exhibit 4-8. User input file used by EMBRET.

For the /COUNTY/, /SIC/, /SCC/, and /PLANT/ packets, EMBRET requires an exact match in the appropriate fields. In order for a record to be extracted, it must meet the specified criteria for ***all*** packets included in the EMBRET user input file, so the user should be wary of the possibility of over- or under-specification. As an example of under-specification, facility identification codes are not necessarily unique; in other words, two different facilities in different counties may have the same facility identification code. In order to uniquely identify one particular facility, the user should also specify the FIPS state/county code for the facility in question.

The second required input is the EMBR file to be converted; Table 2-16 describes the EMBR format.

Output Files

EMBRET produces two output files. The first of these, the EMBRET message file (Exhibit 4-9), summarizes input and output file names and total emissions by criteria pollutants for the input EMBR file and output EMAR file. The second output file is the EMAR emissions file (Table 2-17) which will contain either (1) those records matching the specified extraction criteria (if the user requested a subset of the data in the EMBRET user input file), or (2) all records from the original EMBR file (if no user input file was specified). Exhibit 4-10 provides an example job script for the EMBRET utility.

```
              EPS3 EMBRET utility v. 1.01 Oct 2004      08/09/07 19:01:13


                Input Files
          User input file                :../inputs/embret.input
          Input EMBR file                :../../../embr/embr.cntlem.ar.test_problem


                Output Files
          Output EMAR file               :../emar/emar.embret. ar.test_problem



Number of /COUNTY/ records read:        1
Number of /SIC/ records read:        0
Number of /SCC/ records read:        0
Number of /PLANT/ records read:         0
Number of /SUBGRID/ records read:        0
Number of input EMBR records read:    12293
Number of output EMAR records written:       56


                  Total Emissions Processed
                       English Tons


                       NOX          CO         VOC
    ----------------------------------------------------------
    Input Emissions       585.8311    979.4699   1825.9321
    Output Emissions        0.0681      0.7862      5.6106
    ----------------------------------------------------------
```

Exhibit 4-9. Example of an EMBRET message file.

```
#!/bin/csh
#
#   --- Sample job script for running the
#       EPS3 module EMBRET
#
set EXEC = /models/eps3/src
#
set SCENARIO = test_problem
#
rm -f ../msg/msg.embret.cntlem.ar.$SCENARIO
rm -f ../emar/emar.embret.cntlem.ar.$SCENARIO
#
echo "-------------------------------------------------"
echo "    Running EMBRET for $SCENARIO "
echo "-------------------------------------------------"
#
$EXEC/embret/embret << IEOF
USERIN file         :../inputs/embret.input
Input EMBR file     :../../../embr/embr.cntlem.ar.$SCENARIO
Message file        :../msg/msg.embret.cntlem.ar.$SCENARIO
Output EMAR file
:../emar/emar.embret.cntlem.ar.$SCENARIO
```

Exhibit 4-10. Example of an EMBRET job script.

4.4 SPLTEM

In order to get a better understanding of SPLTEM it is recommended that you review the EMSCVT utility at the beginning of this chapter. EMSCVT and SPLTEM share many of the same input files. EMSCVT generates factors to be applied to an emissions inventory in order to calculate modeling compounds (OLE, PAR, etc) while SPLTEM outputs individual hydrocarbon species (propylene, ethylbenzene, etc).

The SPLTEM utility generates ASCII formatted files of hourly, gridded emissions (grams/hour) of individual hydrocarbon species (calculated from criteria VOC or TOG) and non-VOC criteria pollutant emissions (CO, NOx, etc). The program reads a gridded, temporally allocated, 'compressed'-EMBR file that is produced by the EPS3 GRDEM module when the 'COMP' output format is specified in the /GRDEM/ packet of the USERIN file (refer to Table 3-37). The output EMBR file only includes criteria pollutants, thus the 'compressed' reference, in order to reduce the file size. The criteria VOC/TOG emissions are speciated using the SCC-profile cross reference, the profile definitions (weight fractions of species), and the compound database.

In order to reduce the size of the SPLTEM output files a sub-domain can be specified in the USERIN /SPLTEM/ packet. The SPLTEM utility reads an emissions inventory input record and determines if the grid cell is within the user specified region of interest. If it is, it matches the FIPS/Facility/Stack/SCC codes to a speciation profile code, applies the corresponding weight fractions of the profile, and totals the emissions by hour and grid cell.

Input Files

The SPLTEM utility requires five input files: the user input file USERIN, a gridded temporally allocated compressed EMBR file of emissions, the speciation profile definitions of weight fractions, the SCC(ASC)/speciation profiles cross-reference file, and the compound database used to generate the split factors file by the EMSCVT utility. Exhibit 4-11 provides an example job script for the SPLTEM utility.

```
#!/bin/csh
set EMBR = ../outputs/pts_eastman/embr
set TMP = ../outputs
set INPUT = ../inputs

set RUN = etcog.pts.eastman.040618
set VER = qa01
#==============================================================================
date
echo
echo '--------------------------------------------------------------------'
echo "                      SPLTEM run"
echo '--------------------------------------------------------------------'
echo

rm -f  $TMP/msg.spltem.$RUN.$VER
rm -f  $TMP/spltem_lo.$RUN.$VER
rm -f  $TMP/spltem_el.$RUN.$VER

../src/spltem/spltem.tx << IEOF
USERIN file        :$INPUT/userin.eps3.pts.eastman.wkd_comp
Input embr         :$EMBR/embrcomp.etcog.pts.eastman.040618
Weight fract. file :$INPUT/prof.emscvt.stars_2005_v4a.pt
SCC/VOC Xref       :$INPUT/xref.voc.eps3f.stars_2005_v4a.pt.FACILITY
compound database  :$INPUT/compound.datab.eps3.cb5.wTOG.Nov30.2007
Output message     :$TMP/msg.spltem.$RUN.$VER
output lowlev dat  :$TMP/spltem_lo.$RUN.$VER
output elev dat    :$TMP/spltem_el.$RUN.$VER
IEOF
```
Exhibit 4-11. Example of SPLTEM job script.

SPLTEM reads the /SPLTEM/ packet from the USERIN file. Refer to Exhibit 4-12 for an example of this packet. This packet specifies the input and output hydrocarbons (VOC or TOG). Because emissions inventories can report the mass of organic compounds differently (VOC or TOG), SPLTEM, like EMSCVT, must account for how the input hydrocarbon emissions are reported. Similarly, air quality modeling emission inventories can be prepared as VOC or TOG and SPLTEM provides the option of selecting whether the output hydrocarbons will be calculated as VOC or TOG. You should select the VOC/TOG options based on the type of data included in the initial inventory (AFS and AMS) work files, and the compounds you wish to include in the output speciated emissions file. Typically, input emissions are reported as VOC and modeling is based on TOG. Table 4-10 specifies the /SPLTEM/ packet parameters and formats.

> Note: You have the option of generating ONLY gridded criteria pollutants. This is accomplished by leaving the /SPLTEM/ packet input emissions flag blank (variable LVOCIN). By not specifying a criteria pollutant to split only criteria pollutants are output, including total VOC (or TOG). A blank field will guarantee that no speciation occurs.

```
-----------------------------------------------------------------------
This is the packet that defines the subregion to extract for
the SPLTEM module.

Line 1: 1-20 label (ignored)
Line 1: 21-30 criteria pollutant to split
Line 2: 1-20 label (ignored)
Line 2: 21-30 output splits for
Line 3: 1-20 label (ignored)
Line 3: 21-30 subregion to extract lower left corner X
Line 4: 1-20 label (ignored)
Line 4: 21-30 subregion to extract lower left corner Y
Line 5: 1-20 label (ignored)
Line 5: 21-30 subregion to extract upper right corner X
Line 6: 1-20 label (ignored)
Line 6: 21-30 subregion to extract upper right corner Y
Line 7: 1-20 label (ignored)
Line 7: 21-30 acceptable profile weight range (will be renormalized)
               optional input, default is .05


/SPLTEM/
Criteria to split  : VOC
Output splits      : TOG
Lower Left X       : 1
Lower Left Y       : 1
Upper Right X      : 50
Upper Right Y      : 60
tolerance          : 0.02
/END/
```
Exhibit 4-12. Example of /SPLTEM/ packet.

Table 4-10 /SPLTEM/ packet parameters and formats.

Line	Variable	Columns	Type	Description
1		1-20		Not used
	LVOCIN	21-100	C	Flag to specify input emissions types. options are: VOC = input emissions are VOC TOG = input emissions are TOG blank = do NOT speciate hydocarbons
2		1-20		Not used
	LVOCOUT	21-100	C	Flag to determine generated hydrocarbon species type: VOC = compute emissions as VOC TOG = compute emissions as TOG
3		1-20		Not used
	ILLXCL	21-30	I	Subregion lower left corner X cell index.
4		1-20		Not used
	ILLYCL	21-30	I	Subregion lower left corner Y cell index.
5		1-20		Not used
	IURXCL	21-30	I	Subregion upper right corner X cell index.
6		1-20		Not used
	IURYCL	21-30	I	Subregion upper right corner Y cell index.
7		1-20		Not used
	EPSLON	21-30	R	Range used to determine a valid profile weight, default is 0.05.

The SPLTEM packet also includes coordinates of a rectangular subregion to examine and process. The parameters are the lower left corner X and Y grid cell indices and the upper right corner X and Y grid cell indices (inclusive).

The final /SPLTEM/ packet input is a tolerance parameter. This parameter determines the range of values SPLTEM will accept for a correct profile weight. The absolute value of one minus the sum of all weight fractions for a profile must be less than this value in order for the profile to be acceptable. If the tolerance parameter is exceeded, SPLTEM renormalizes the weight fractions. This option can be used to ensure that all weight profiles are complete. However, because of roundoff issues it is often difficult to get a profile that adds exactly to one. The tolerance value determines how much roundoff is acceptable. The default is .05.

The second input file is the gridded temporally allocated compressed binary EMBR file. Only the criteria pollutant emissions are available in this file format, thus it is referred to as 'compressed'. The EMBR header records provide the size and parameters of the modeling domain grid. If the file is not gridded then processing will stop with an error message to inform the user that the record is not gridded.

The third input file, the weight fractions data defines the composition of each profile. This file contains profile code, AIRS pollutant code and weight fraction for each chemical compound/species. Refer to Table 4-3 and Exhibit 4-2 in the description of EMSCVT for the file format specification.

The SCC(ASC)/speciation profiles cross-reference file uniquely identifies which speciation profile is required for each emission source. Refer to the CHMSPL module Exhibit 3-23 and Table 3-19 for an example and file format. The source is identified by FIPS code, facility identification codes (for point sources), and SCC(ASC) code. For this reason, *it is not necessary to create new SCC codes for point sources with unique speciation profiles*. It is sufficient to create additional cross reference records with the plant id and stack id of the indicated point source, making sure that each unique source has a unique plant/stack id profile.

The final input file is the compound database that was used to generate the split factors file for CHMSPL speciation. This file format is described in detail under EMSCVT, Table 4-4 and Exhibit 4-3. The compound database provides a mapping of chemical species in the weight fractions file to modeling compounds. The SPLTEM utility extracts two pieces of information from this file; the species name which is used for reporting purposes and the VOC reactivity flag which is used in converting VOC to TOG.

It is important that the same parameters and input files be specified for the SPLTEM utility as were specified for EMSCVT. This is necessary to ensure that profiles and speciation are treated the same in the modeling and the reporting.

Output Files

SPLTEM produces three output files: a message file summarizing the SPLTEM utility processing, a file of emissions for the user specified region of interest for low-level sources, and optionally a file of emissions in the user specified region of interest for elevated point sources.

The output message file summarizes the SPLTEM utility processing. It includes utility name, list of input and output file names which the user has specified, modeling grid parameters extracted from the EMBR header records, input and output hydrocarbon specification, grid cell boundary of the specified subregion, user specified profile tolerance, number of new SCC/profile records found in the profile definitions file (this is a standard message from the called library routine when a profile is read), number of EMBR records read and processed, an emissions summary table of criteria pollutants processed, and an emissions summary table by profile code. Exhibit 4-13 is an example SPLTEM output message file. In addition, the message file will contain any warning messages that occur during processing.

```
                    EPS3 SPLTEM utility v. 2.00 Feb 08

         Input Files
    USERIN file                  :../inputs/userin.eps3.mv.etcog.04km_noTX.wkd
    Input compressed EMBR file   :../outputs/embrcmp.etcog.mv.04km.noTX.wkd
    Weight fractions file        :../inputs/emscvt.mobile_profiles
    ASC-SCC/profile code xref file:../inputs/chmprf.xref.voc.MV_hstn_upd.m6.evp
    Compound database file       :../inputs/compound.database.eps3.cb5.wTOG.Nov30.2007

         Output Files
    Output data file             :../outputs/spltem_lo.etcog.04km.noTX.wkd
    Output elevated data file    :../outputs/spltem_el.etcog.04km.noTX.wkd

            EPS3 SPLTEM utility v. 2.00 Feb 08      02/27/08 09:30:17

         Extracted from EMBR header
    UTM origin (km)              : ( 396.00,-900.00)
    UTM zone                     :    0
    Grid cell width (km)         : (   4.00,   4.00)
    Number of cells              :   54   45

    Criteria pollutant to split  : VOC

    Output HCs specified as      : TOG

    Grid cell boundary of region to extract -
    Lower left corner            : XY ( 556.00,-820.00)  IJ (   40,   20)
    Upper right corner           : XY ( 596.00,-720.00)  IJ (   50,   45)

    Specified tolerance          :    0.020
Number of new ASC-SCC/profile cross reference records for profile: H2K2S              0
Number of new ASC-SCC/profile cross reference records for profile: H2KGS              0
…
Number of new ASC-SCC/profile cross reference records for profile: D411               0

         Number of weight fraction profiles read:     11
         Number of input records read:   534102
         Number of input records outside region of interest:   254537
         Number of lowlevel input records:   279565
         Number of elevated input records:         0
         Number of skipped input records:         0
         Number of input records written for output:   279565

                         Total Emissions Processed
                              English Tons
                    NOX          VOC          CO          SO2
  ------------------------------------------------------------------------------
  Input Emissions     28.2289      18.1988     199.0696       0.
  Output Emissions    20.1598      13.9234     149.0676       0.
  Low Level Emissions 20.1598      13.9234     149.0676       0.
  Elevated Emissions     0.           0.           0.          0.
  Emissions Skipped      0.           0.           0.          0.
  Outside Sub Region   8.0778       4.2940      50.0743       0.
  ------------------------------------------------------------------------------


 Output Emissions by Profile Code
         English Tons
     Profile          VOC
  ---------------------------------
  H2KGV              6.5688
  H2KWT              6.8453
  D201               0.5135
  ---------------------------------
```
Exhibit 4-13. Example of the SPLTEM output message file.

The hourly, gridded emissions within the specified subregion are written to a formatted ASCII file. This file contains hour, I grid cell, J grid cell, pollutant code, emissions value (grams per hour), and the pollutant name (if included as part of the compound database). The pollutants include the individual hydrocarbon species as well as the non-VOC criteria pollutants. Refer to Exhibit 4-14 for an example of the output file.

```
 0  28  24 43203 0.1194E+04 ethylene
 0  28  24 43204 0.2151E+03 propane
 0  28  24 43212 0.6242E+02 n-butane
 0  28  24 43122 0.8520E+00 isomers of pentane
 0  28  24 43214 0.3778E+01 2-methylpropane; isobutane
 0  35  26 43302 0.7074E+02 ethyl alcohol
 0  35  26 43433 0.2120E+03 ethyl acetate
 0  30  28 42603 0.1134E+01 NOX
 0  30  28 42101 0.3780E+00 CO
```

Exhibit 4-14. Example of the output gridded emissions file; hour, Icell, Jcell, pollutant code, emissions (grams/hour), pollutant name.

A second, optional, output file can be generated for elevated point sources. If the input EMBR file contains elevated point sources (which are flagged internally by the PREPNT module) then these sources will be written to the second output file **only if** the user supplies a valid file name in the job script. If no output file is specified for elevated sources and the input EMBR file contains elevated sources then the elevated points are not output. They **do not** default to the low level output file.