

Processing Emission Inventory Data in the Models-3 Integrated Distributed Modeling System: A Tutorial Example

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ABSTRACT

This paper presents a brief tutorial example and describes the benefits of emission inventory data processing for air quality modeling using the windows of the Study Planner of the Models-3 environmental modeling system. The functions of the key windows and the procedure for using them are illustrated using a 21 column by 21 row spatial grid with 12 km cell resolution, centered on Birmingham, Alabama. The Study Planner makes manipulation of input data and processing programs relatively simple and flexible. Emission inventory processing that had often been accomplished step-by-step with large amounts of intensive labor, including quality control, spatial allocation (gridding), temporal allocation, and chemical speciation, has now been automated. It is not necessary to change processor coding for different study areas, spatial resolutions, and time, to remember the locations of data files and processors in the system, and to use command line instructions to initiate and control the processing system for each step.

INTRODUCTION

The processing of air pollutant emission inventory data for use in urban and regional scale air quality modeling is often complicated and time-consuming. For each study area, processing typically requires conversion of different inventory formats to a consistent format, painstaking but time-limited quality control of the emission data, and spatial, temporal, and chemical species allocation of the data. These steps are often accomplished independently, which increases the likelihood of data errors and inconsistencies between steps. The Models-3 Emission Processing and Projection System (MEPPS) integrates and substantially automates emission data processing and quality control, reducing the chances for undetected errors. Models-3 is a distributed environmental modeling framework, initially focused on air quality modeling.¹ It is designed to integrate modular modeling components (including MEPPS), automatically track files with metadata, simplify data processing and model setup and execution, enable the use of consistent data formats between system components, and provide a suite of visualization analysis tools. Models-3 runs on Sun® UNIX-based workstations, and will be ported to other UNIX and Windows NT® based machines in the future. The emission projection capability runs on both UNIX-based workstations using Soft Windows®, and Windows NT®. The purpose of this paper is to illustrate the operation and benefits of MEPPS processing of a base year inventory through a tutorial example. The operation is described in sequence. However, description of all specific steps and options is beyond the space limitations of this paper. More detailed information is available in the draft Models-3 User Manual and Tutorial.²

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Benefits of the Models-3 Emission Processor

Compared with previous practices, processing emission inventory data with Models-3 offers several significant benefits. These reduce overall processing and personnel time. The following principal benefits are illustrated by the discussion of the processing system in this paper.

- The system, including the emission processor, is relatively easy to use and flexible. Clear menu windows with pick lists, help buttons, and selectable icons are used for navigation, modification and option selection, and for execution of processing. Changes in options and files do not require recoding or command line instructions.
- Repetitive processing is more efficient. Once a processing sequence is established, processing may proceed with little human supervision; and minor changes between processing runs are made simply through the windows.
- Management of emission files and programs within the system is simplified. The Models-3 File Manager tracks all registered files through associated metadata, and newly created files are automatically named and tracked by an internal convention. Consequently, file access is easy and old files are not inadvertently overwritten.
- Processed emission inventory data are directly available in a common format and in common locations for use in air quality modeling or other applications in the Models-3 system. Reformatting or maintaining duplicate data files are not necessary within the system.

Emission Processor Structure

Figure 1 illustrates the key role of MEPPS as a module within the Models-3, along with the meteorology data generated by Mesoscale Model 5 (MM5) (through the Meteorology Chemistry Input Processor or MCIP) and the Community Multiscale Air Quality (CMAQ) model. The meteorology data are input for both MEPPS and CMAQ, and MEPPS provides processed emission data to CMAQ. Data are passed between modules in NetCDF format using the Models-3 Input/Output Applications Program Interface (I/O API).³ The MEPPS is a SAS[®]-based system which incorporates the ARC/Info[®] geographic information system (GIS) to accomplish spatial allocation of either discrete point source emission data or data derived using surrogate spatial information (area, mobile, and biogenic sources). The core of MEPPS is a greatly modified version of the Geocoded Emission Modeling and Projection (GEMAP) system⁴ (now known as the Emission Modeling System 95 (EMS-95)).

The major internal components of MEPPS are shown in Figure 2. The input processor (INPRO) inputs and quality controls emission inventory and meteorology data, and reformats and subsets the inventory data to the spatial domain specified by the user. The main processor (EMPRO) is the portion derived from GEMAP. The EMPRO allocates point, area, mobile, and biogenic emission data spatially (by grid cell) and temporally (by time step) according to user specifications. It also chemically speciates the emission data using source-category specific species split factors associated with either the Regional Acid Deposition Model (RADM) 2.0,⁵ Carbon Bond 4 (CB4) chemical mechanisms,⁶ or a generic speciation mechanism modifiable by the user. Mobile and biogenic source emissions for the period of interest are estimated within EMPRO which runs the Mobile 5a⁷ and BEIS-2⁸ models, respectively. With user-defined criteria, OUTPRO merges specified EMPRO-processed point, area, mobile, biogenic source files into a file of surface emission data, and a file of elevated point source stack emission data. These files are converted to the NetCDF I/O API format and provided as modeling input to CMAQ. The OUTPRO also provides standard and user-defined summary and quality control output files.

Basic Functions

Figure 3 shows the main window of the Models-3 system. Each icon accesses a high-level function of the system. The key functions to process emission inventory data using the Models-3

windows are in the Science Manager, Study Planner, and Strategy Manager. The MEPPS may also be accessed through the Tool Manager using SAS® screens for detailed interactive use of the processors, editing of input and lookup files, access to intermediate files, and selection of specific non-standard options. However, many of the advantages of using Models-3 for emission processing are associated with the use of Study Planner windows, which is the approach addressed here. Study Planner is perhaps the key feature of Models-3. It allows the use of selectable icons on an interactive screen to define and link component models, properties, data files, and tools; and to execute defined actions such as estimating biogenic emissions. A study is any environmental analysis activity or sequence of activities defined by the user in Study Planner. A study may consist of several plans. A plan is a smaller sequence of activities that may be a subset of a study. Typical studies and plans (described later) have been established under tutorial study "tutebase" in the Study Planner for the main components of emission data processing (point, area, mobile, biogenic, and output processing). These plans call scripts, which each link a series of processing programs. The existing plans may be modified (annotated) to link to input and output data of interest and appropriate environment variables, which is usually sufficient to process emission data. This approach avoids the need to modify or separately run each program for each emission study.

Science Manager establishes new, and provides access to existing, user-defined coordinate systems and spatial grids, vertical coordinates, and (soon) definition of specific dates of interest (cases). Strategy Manager accesses the Models-3 Emission Projection Processing System (MEPRO). The MEPRO projects base year emission data using source-category-specific economic growth factors and then sends (either interactively or automatically by a defined plan) the projected inventory to EMPRO for modeling pre-processing.

EMISSION PROCESSING USING STUDY PLANS

The example used in the figures in the following sections was prepared as a tutorial for Models-3. The spatial extent includes most of Alabama and part of Mississippi, using 12 km grid cell spatial resolution with 21 cell rows and 21 cell columns (Figure 4). The case (date) chosen is July 27, 1988. The processing sequence followed begins with annual emission inventory data, spatially allocates the data from a point source or area (usually county-level) basis, temporally allocates emission data to time steps needed for air quality modeling, chemically speciates emission data to the species grouping needed for modeling, and outputs files in NetCDF I/O API format.

Accessing Input and Output Data

Input data files (emission inventories, meteorology data) needed within Models-3 are registered by the system using user-supplied metadata (descriptive data about the files) through the File Manager. Once registered, the data files may be easily located and referenced by name or key word searches without typing in their specific location from memory. Input files for emission processing are specified when defining data links in a study plan in the Study Planner windows. Study output files are automatically named and registered by the Models-3 system when created. Input files are generally located in the directory structure "\$M3_DATA/datasets/nostudies", and output files are automatically named and registered in "\$MODELS3/datasets/studies/*study_acronym/plan_acronym/run_number/program_acroynms/logical_name/user_id-unique_number*", where italicized names are variable by study. \$M3_DATA and \$MODELS3 are environment variables defined by the system administrator to represent file locations on a computer system.

Description of Window Functions

The following paragraphs describe access to and contents of the principal Study Planner windows, from general to specific, which are used to process emission inventory data using existing emission processing study plans. The user may also use the windows to generate new study plans using new or existing components. Principal windows include generic menu and generic tool bar

icons at the top. The icons, from left to right (see Figure 5), represent new, open existing, save, print, undo, detail (of existing selection, help, and exit. Space limitations preclude showing all windows.

- The Study Planner icon is selected using a mouse from the main Models-3 window.
- The Study Planner (Figure 5) provides the name and brief description of studies from which to select. If the study of interest is not listed, the Find Study icon (a file folder in the tool bar at the top of the screen) is selected which can search by key word. If a new study is needed, the white page icon (new) is selected to access a blank series of study and plan screens to use in defining the study. For this example, the existing study "tutebase" is chosen and you are returned to the Study Planner window.
- In the Study Planner window, the name of the study of interest is selected. The study "tutebase" contains a series of emission processing plans which may be modified and reused. It is highlighted and a "S" (selected) appears in the left margin.
- The "detail" button (eye and lens icon) is selected next. A window containing four overlapping tabbed windows appears. The Study Properties window appears on top (Figure 6) listing the study name, acronym, description, and the environmental variables related to the study. These properties are tracked automatically once entered.
- The "Plans" tab invokes a window listing the plans included within the specified study (Figure 7). Each plan is an ensemble of programs and datasets which may be executed from the Study Planner. There are separate plans for processing point, area, mobile, and biogenic source emission data through chemical speciation, and a plan for merging and reporting emission processing output data. The area source processing plan is highlighted.
- The tab for the Environmental Parameter window (not shown) displays a list of the environmental variables associated with the plan. These variables are automatically copied from the study level, and may be edited, deleted, or inserted from the Environment Variable window.
- The Plan Layout tab is selected next. A window with selectable icons, including process node icons (rectangles) and data dependency links (arrows) of the plan, appears (Figure 8). The dependencies refer to the logical and physical file names and locations. The icons down the left side are used to create or modify a plan. A plan may be defined, modified, and executed from Plan Layout using these icons. It is not necessary to recode any of the information once it exists in the system. A Legend icon on the lower right of the window gives access to a window which specifies the meaning of the selectable icons and their color coding. Buttons along the bottom of the window allow execution, termination, and suspension of execution, and resetting of the screen. "VCR" (video cassette recorder) style buttons allow navigation between plans associated with a study.
- If the user selects a rectangular icon (node), a Node Properties window appears (Figure 9). It displays environment variables for the node and commands and arguments associated with the underlying programs invoked by the node. A program detail icon invokes a window which shows the programs and environmental variables associated with the node. Because there are many underlying programs in MEPPS used in emission data processing, the programs have been linked by scripts and grouped corresponding to point, area, mobile, and biogenic emission processing to reduce the complexity of the Plan Layout windows. Table 1 lists the existing emission processing scripts which are called from the process nodes. The environmental variables may be selected and viewed or cleared, and new variables may be inserted using the Insert window invoked by the View button. The command arguments modify specific programs and may be used to vary the application of the program. For example, the argument for the "extract.ar" program script used to extract inventory data for area source processing may be varied to reference different inventories (e.g., 90, 95).
- From the Plan Layout window, a link arrow is selected by double-clicking on it. A Link

Properties window appears which lists the "from" and "to" processing data dependencies by name and location in the Models-3 system. It is not necessary to examine file formats and contents for consistency and quality at this stage. The quality control was performed when data was imported to the system, and Models-3 provides an internal standard for data format. An Insert button will invoke a window which allows entry of command arguments, environmental variables, or input data files (Figure 10).

Processing Procedure

Processing of emission inventory data is accomplished by executing properly annotated study plans from Plan Layout windows for point, area, mobile, and biogenic emissions. The example study also includes a plan for reporting, merging and format conversion of emission output files in OUTPRO. For each plan, the study case (time period) is defined by specifying environment variables for the year and start and stop times. Case will be defined from Science Manager in the public release expected in July, 1998. The sequence of processing in each plan is similar, as illustrated by the order of the nodes.

The area source emission processing plan (Figure 8) and point source plan (Figure 11) both extract data from an inventory (first node), load the data (second node), grid the data (third node), calculate the emissions by county (fourth node), and speciate the emission data (fifth node). Environment variables are used to specify the inventory, spatial grid to be used, and the speciation split factor mechanism (specifics on the environment variables are in the user's manual).

The biogenic source emission plan (not shown) includes two nodes for calculating the emissions and for speciating the data. In addition, biogenic and mobile source emission processing require meteorological data processed by MCIP. Existing meteorology data files are presently extracted in advance of plan execution by using the MEPPS INPRO interactively. The first public release will include additional nodes in the standard biogenic and mobile source plans which extract the meteorology data as part of plan execution.

The mobile source emission plan (Figure 12) includes nodes for inventory data extraction (vehicle miles traveled data, or VMT), loading of data, gridding of data, computation of emissions by county using Mobile 5a-generated emission factors, and speciation. Prior to plan execution, the user must specify the geographic location of specific information for fuel use, Inspection and Maintenance Programs, and fleet structure in a lookup file (m5a.mv) located with other lookup tables in the common directory established for the study. Models-3 provides a template for the lookup file. A mobile source particulate emission model (PART 5)⁹ will be included in the initial public release. New gaseous and particulate mobile source models will be incorporated into MEPPS as soon as they are available, possibly in late 1998 and 1999, respectively.

Processed emission data from the point, area, biogenic, and mobile plans must be merged and placed in the NetCDF I/O API format before use in modeling. The output processing plan (Figure 13), contains a processing node ("define splits") which allows the use of environment variables to define point source criteria for major elevated and major sources (Figure 14). The next processing node creates a file of the selected large point source data for plume rise modeling, including stack parameters and converts the file to NetCDF I/O API. The last node merges the user's choice of area, biogenic, mobile, and minor (smaller) point source files into a single file containing total surface emission data by grid cell, time step, and chemical species group; and performs the format conversion. Merge choices are indicated by "yes" or "no" for inclusion in the node environment variables (Figure 15). The circled dot in the plan is the defined destination of the processed files.

Output Files

The MEPPS produces up to nine output files in NetCDF I/O API format, each with the suffix ".ioapi" (Figure 16). The output files are located at \$EMS_RUN, along with the system log files and error report files. \$EMS_RUN is an environment variable defining the location of the MEPPS output files. The log and error files contain detailed quality control information about the processing and any problems. Only the NetCDF I/O API files are passed to \$MODELS3/datasets/studies/*study_acronym/* for use elsewhere in the Models-3 system.

Quality Control Capabilities

The MEPPS includes a variety of standard and optional reporting capabilities, as well as error messages, designed to improve the quality control of input data and of processing of emission data. The quality control components are accessed by running MEPPS interactively through the Tools Manager. When INPRO extracts annual emission inventory data for a study, it produces, for example, summary tables of the data by political units, pollutant, number of point source stacks, ranking tables of the one hundred largest sources (point or area) in the study area. These reports appear in a log file which may be saved for future reference. In addition, SAS® emission files internal to MEPPS (may be visualized for quality control and analysis by using the Arc/Info®-based visualization tool in EMPRO). The tool contains substantial capabilities for alternate displays, interactive query, and spatial subsetting of emission data. These abilities help locate data inconsistencies that are not apparent from computerized checks for missing files, range checks, and summary tables and statistics.

Emission Projections

Future year emission projections and control strategies are accomplished through the Models-3 Strategy Manager. The Strategy Manager icon on the Models-3 main window establishes a link with the Models-3 Emission Projection Processing (MEPRO) system. The MEPRO is an enhanced version of the Multiple Projection System¹⁰ and uses source-category-specific economic growth factors from the Economic Growth and Analysis System (EGAS)¹¹ and user-specified source-category-specific control factors to project ungridded annual emission inventory data. The MEPRO projects point and area source emission data, and VMT data for mobile sources. Approximate mobile source emission projections can be accomplished by MEPRO. However, more accurate results are obtained by modeling the projected VMT data with the Mobile 5 model in EMPRO. Biogenic emission data can not be projected with economic growth factors because they depend directly upon land cover changes. Projected emission inventory data are passed directly to EMPRO for processing in the same manner as described for base year inventory emission data. A series of alternative control factors may be edited through a table and iteratively applied to projected emissions by MEPRO. The controlled projected emission data are then processed through EMPRO and used in air quality modeling to help provide acceptable alternative strategies to attain ambient air quality standards.

CONCLUSIONS

This paper illustrates some benefits that MEPPS possesses for iterative processing of emission inventory data for alternative control strategy evaluation, and air quality modeling. The principal benefits are ease of use through Study Planner windows, flexibility for use and modification of studies, consistent internal file formats, ease of locating data and program files, ability to quickly perform iterative runs, and the availability of a wide range of quality control reports and analysis tools. These benefits allow more time spent on analysis and less on manipulation of the programs and data.

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DISCLAIMER

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Table 1. Established emission processing program scripts and functions.

Processor program script	Function
mepps_calc_ar	Calculate area source emissions
mepps_calc_bi	Calculate biogenic emissions
mepps_calc_mv	Calculate mobile source emissions
mepps_calc_pt	Calculate point source emissions
mepps_create_stk	Create stack I/O API files
mepps_define_splits	Define stack categories
mepps_extract_ar	Extract area source emissions data from inventory
mepps_extract_mv	Extract mobile source VMT data from inventory
mepps_extract_pt	Extract point source emission data from inventory
mepps_exuser_ar	Extract area source emission data for user defined study area
mepps_exuser_mv	Extract mobile source data for user defined study area
mepps_exuser_pt	Extract point source emission data for user defined study area
mepps_grid_ar	Get area source spatial surrogates for gridding
mepps_grid_mv	Get mobile source spatial surrogates for gridding
mepps_grid_pt	Assign point source data to grid cells
mepps_load_ar	Load area source foundation emission files
mepps_load_mv	Load mobile source foundation files
mepps_load_pt	Load point source foundation emission files
mepps_spec_ar	Speciate area source emission data
mepps_spec_bi	Speciate biogenic source emission data
mepps_spec_mv	Speciate mobile source emission data
mepps_spec_pt	Speciate point source emission data

Figure 1. The position of MEPPS as a module in the Models-3 system.

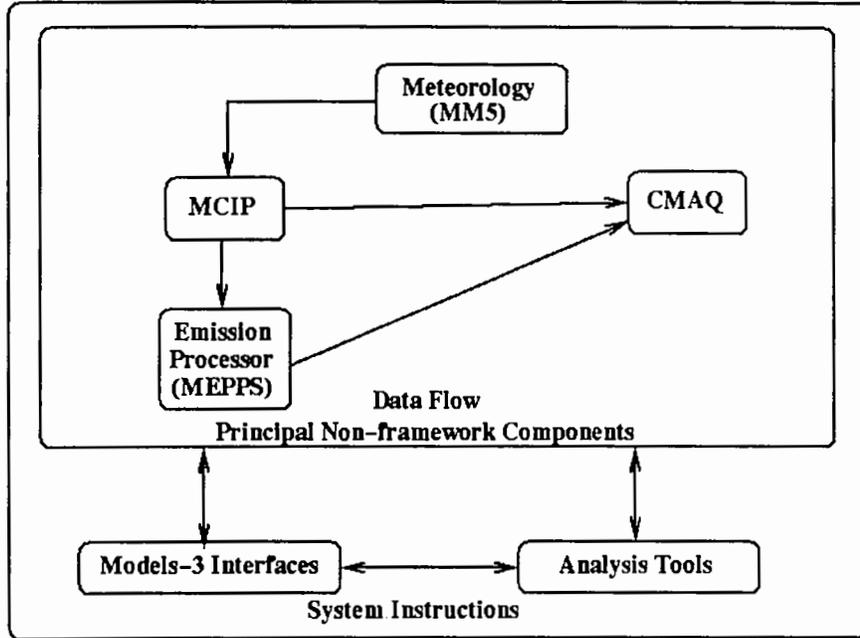


Figure 2. Principal components of MEPPS.

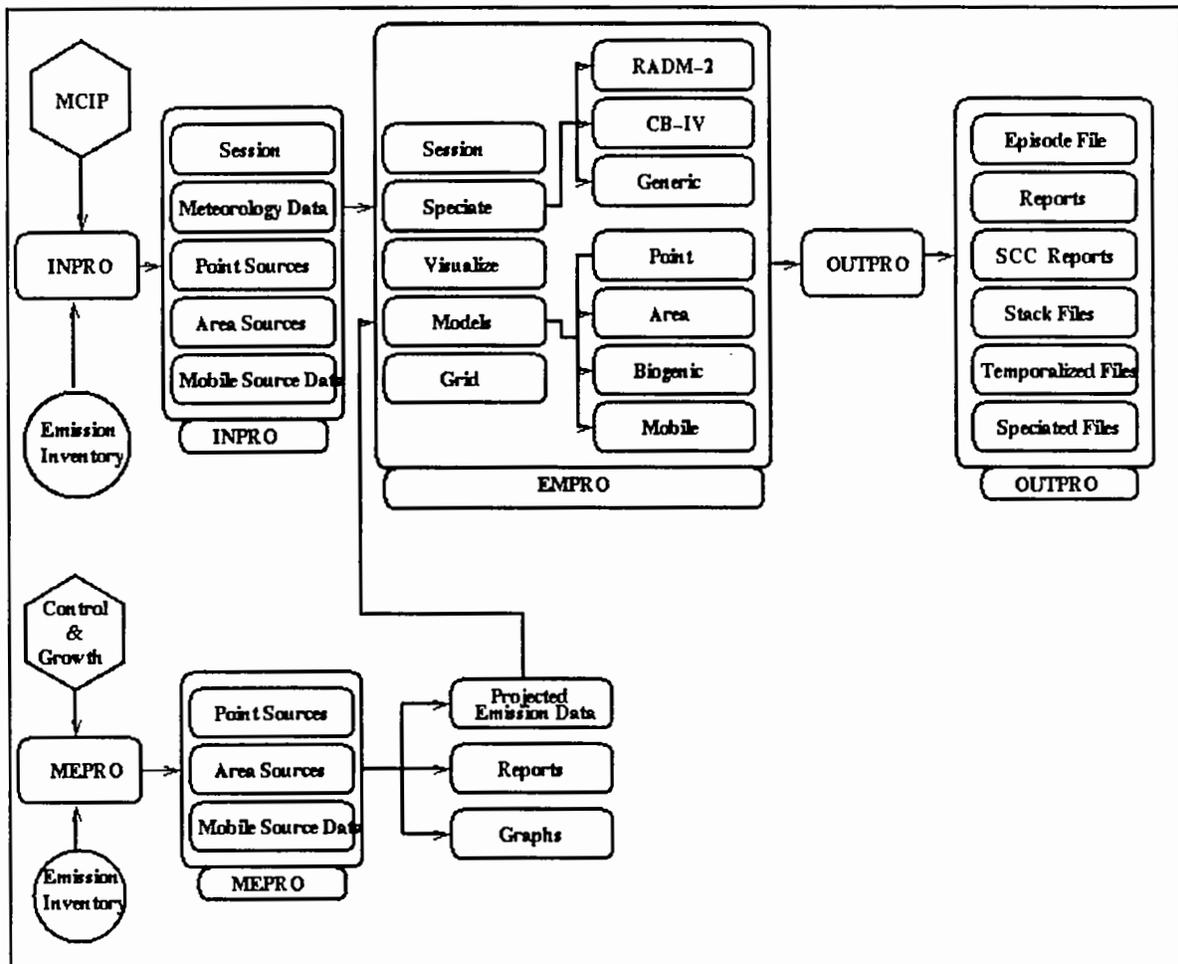


Figure 3. Main Models-3 graphical user interface.

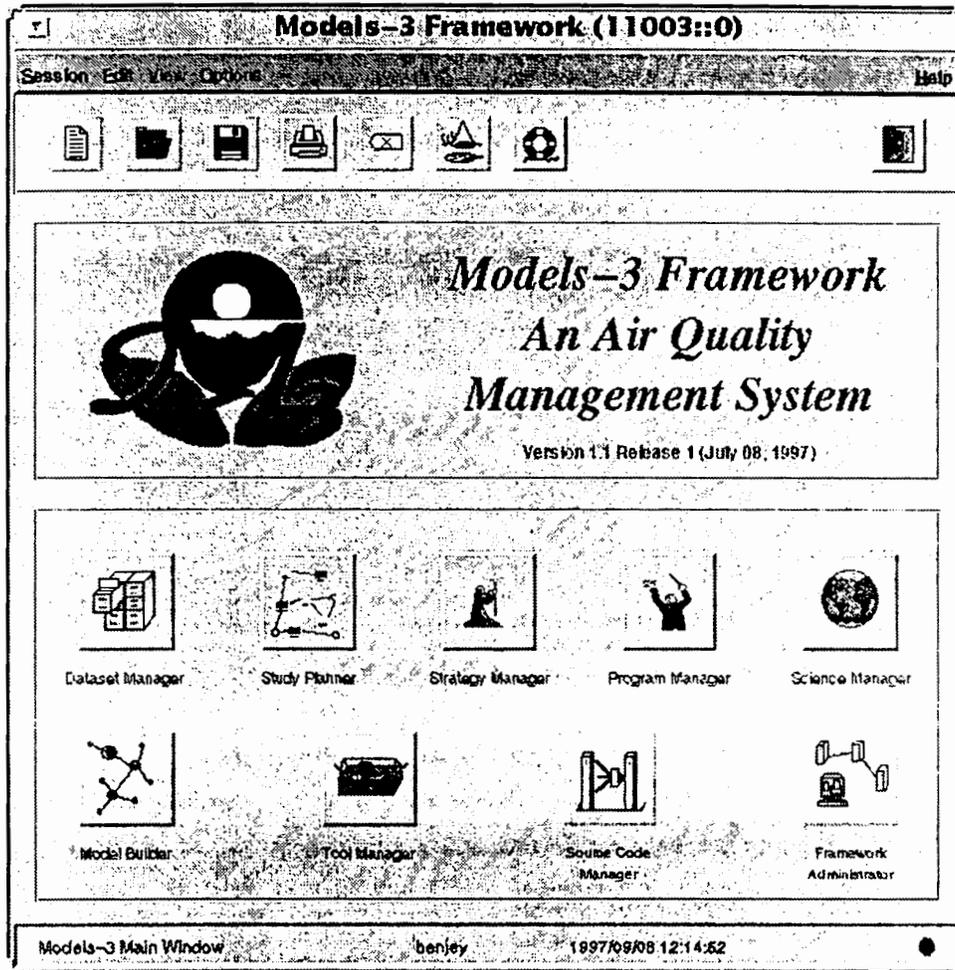


Figure 4. Tutorial grid centered on Birmingham, Alabama, with 12 km grid cell resolution.

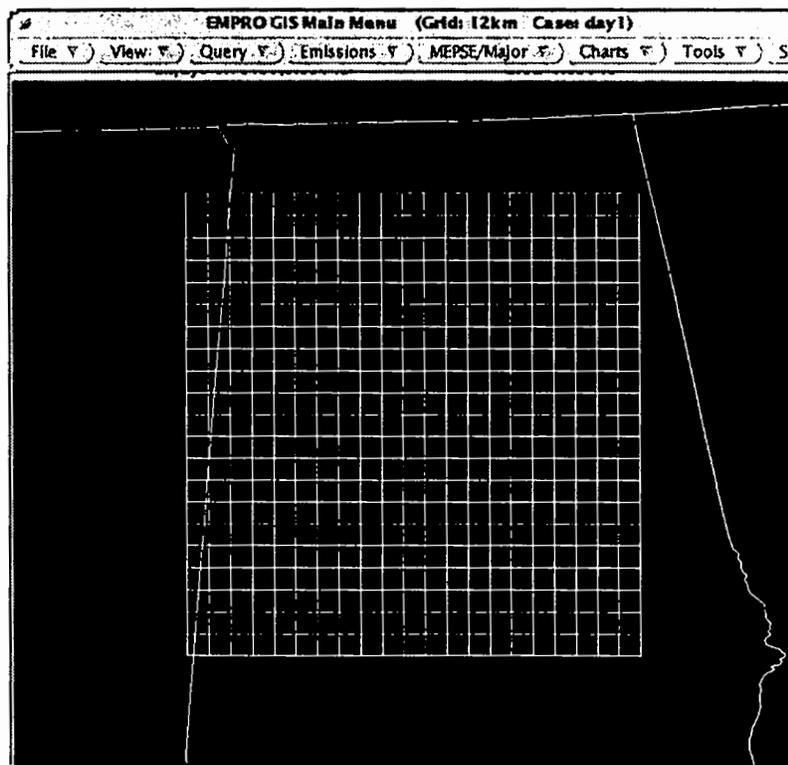


Figure 5. Study Planner window with selected study plan "tutbase".

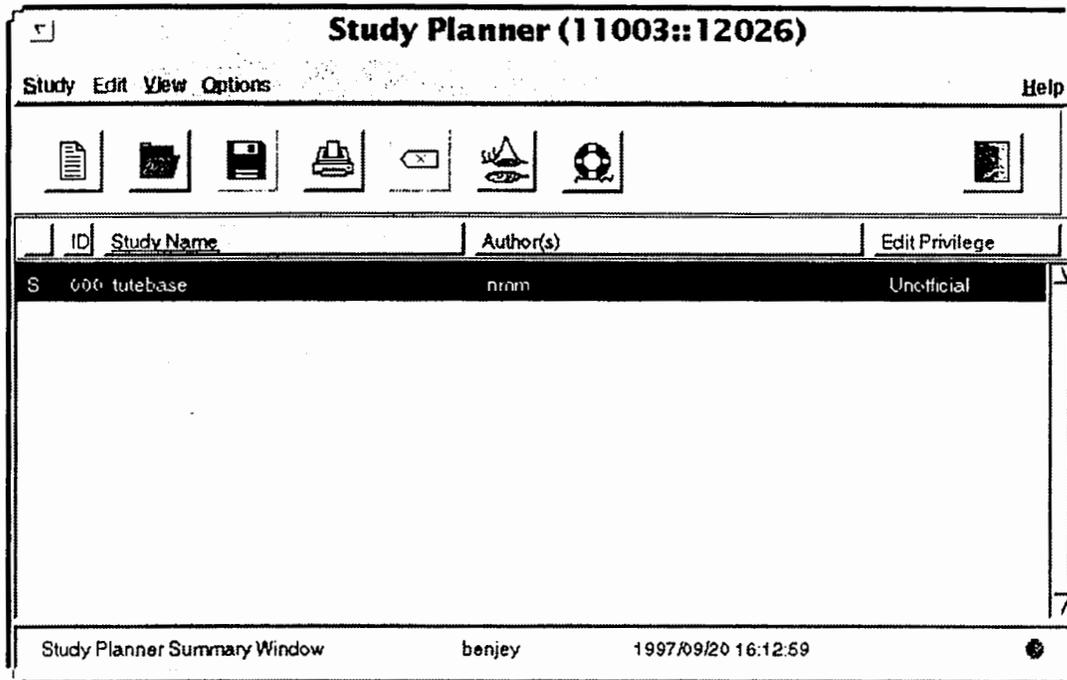


Figure 6. A Study Properties window for an area source emission processing plan under the study planner.

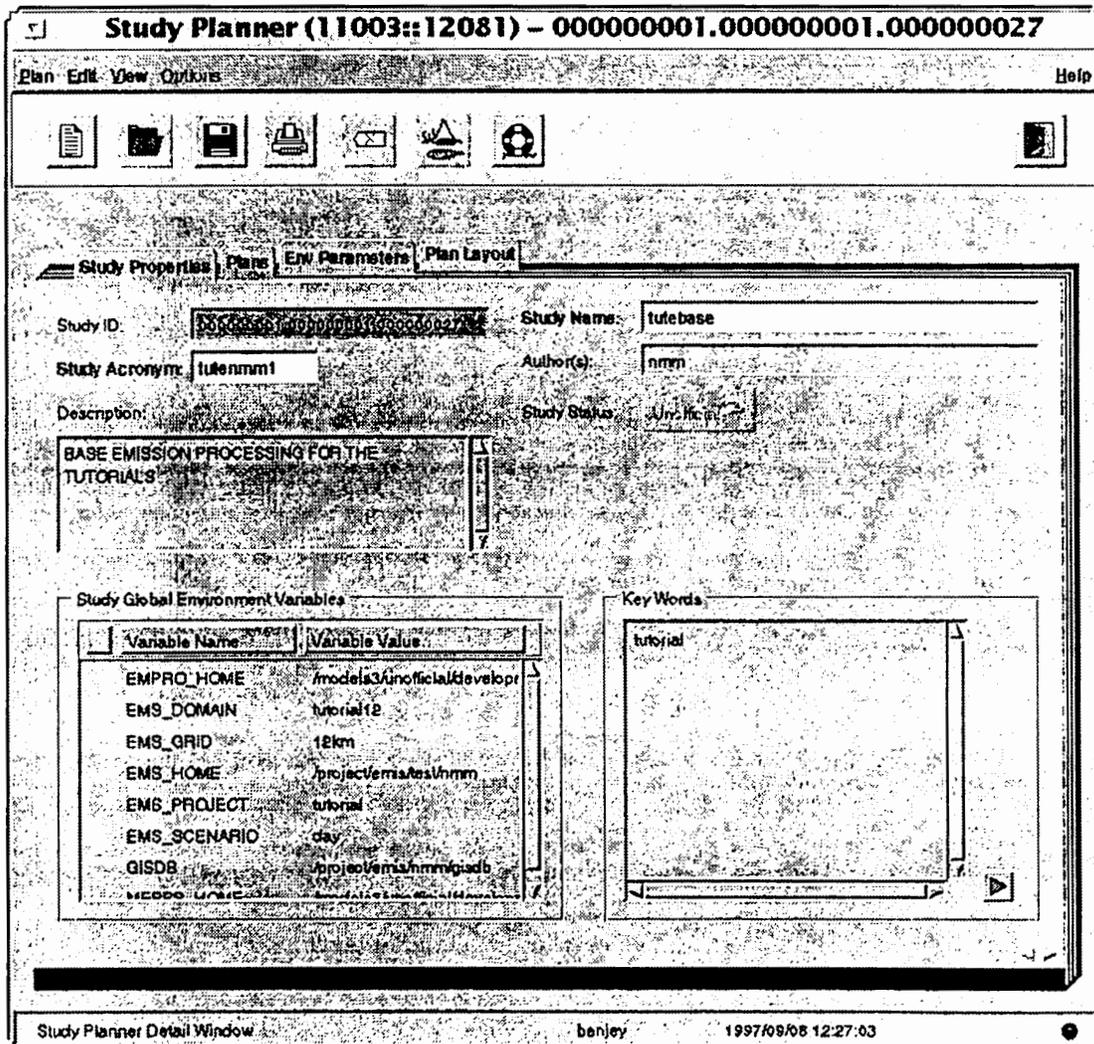


Figure 7. Emission processing plans available in the plan window under study "tutebase".

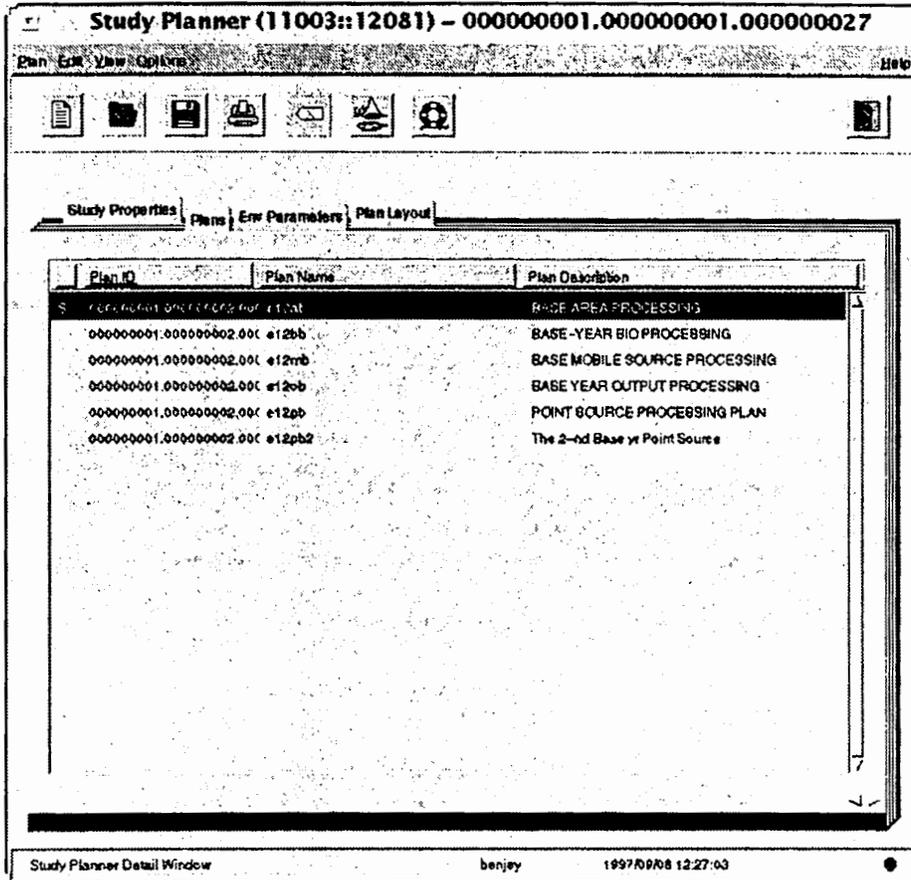


Figure 8. A Plan Layout window for an area source emission processing plan.

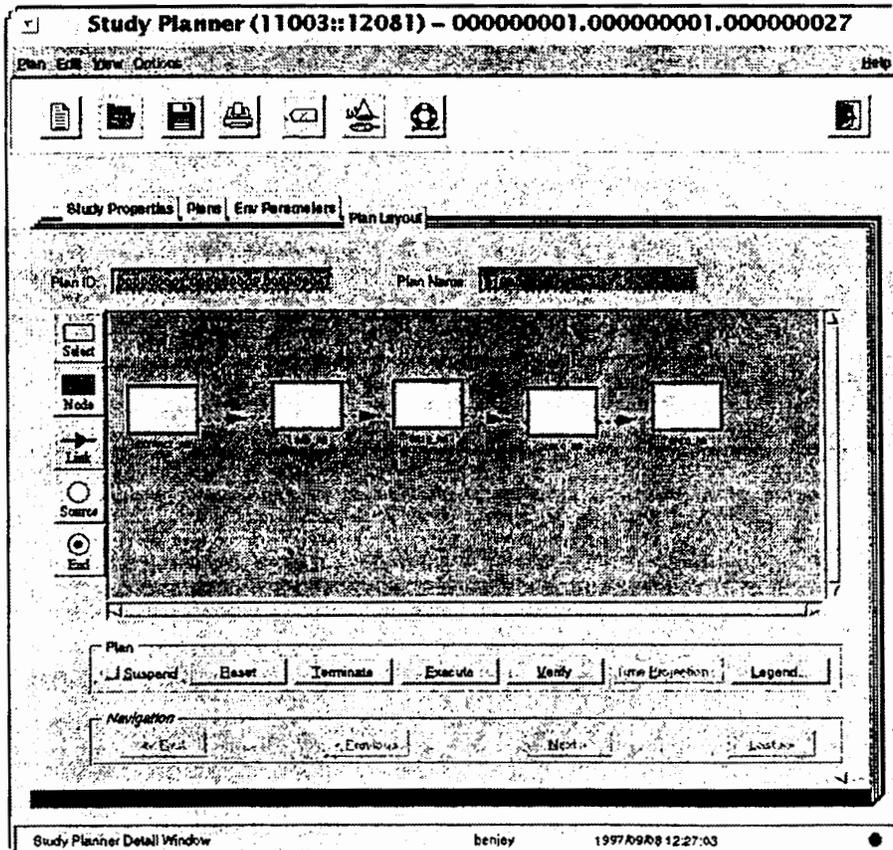


Figure 9. A Node Properties window accessed from a Study Layout node.

Node Properties

Node Name:

Program

Name:

Execution Full Path:

Execution Host:

User ID: Password:

Environment Variables

Variable Name	Variable Value	Description
EMPRO_HOME	/models3/official/development/emp/roA2/	BASE DIR
EMS_DOMAIN	tutorial12	SOURCE
EMS_GRID	12km	GRID ID
EMS_HOME	/project/ems/test/nmm	WORK-S

Command Line Arguments

Argument Name	Argument Value	Description
extract ar	85	Extract fr
extract ar	88	Extract fr
extract ar	90	Extract fr

Cmd Line Arg:

Datasets

Register Save Duration: days

Figure 10. Link Information window used to establish "to" and "from" relationships for links on a Plan Layout window.

Link Information

From Logical Name:

From Physical Name:

To Physical Name:

To Logical Name:

Link as:

Navigation

Figure 11. A Plan Layout window for point source emission data processing.

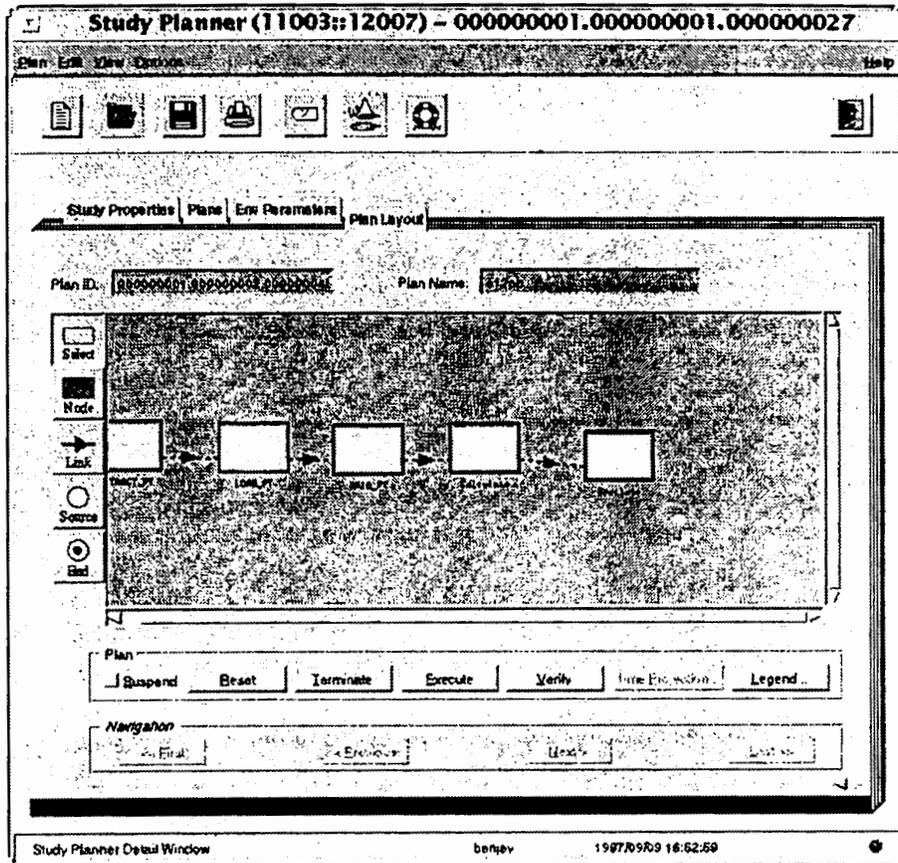


Figure 12. A Plan Layout window for mobile source emission data processing.

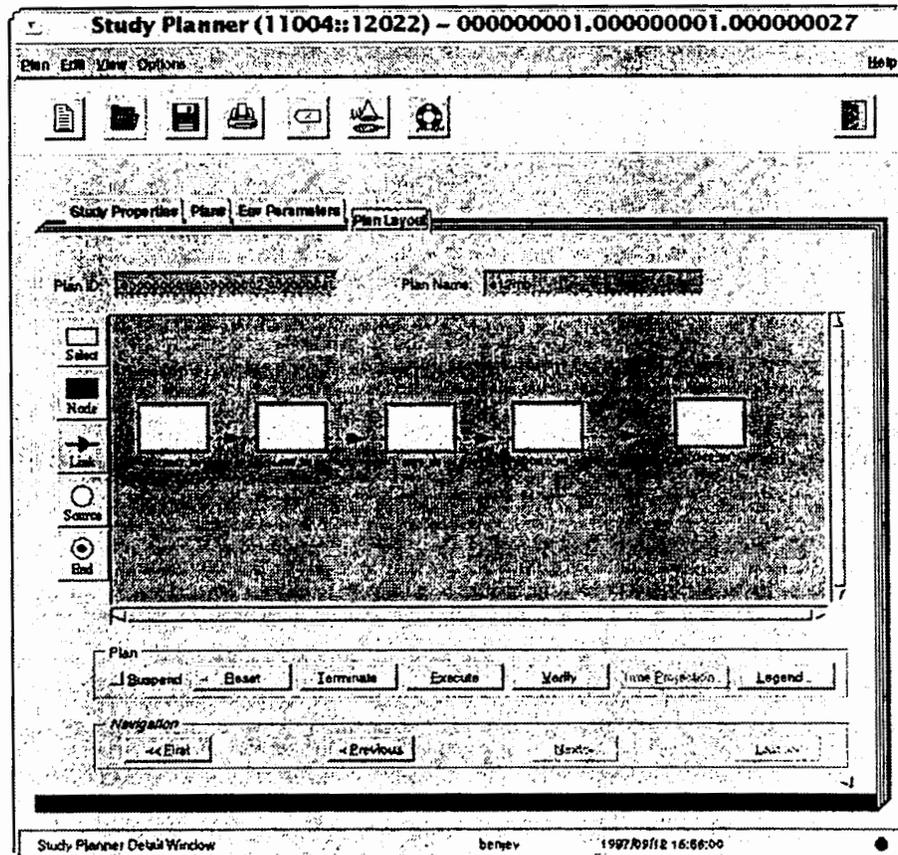


Figure 13. A Plan Layout for output processing of emission data.

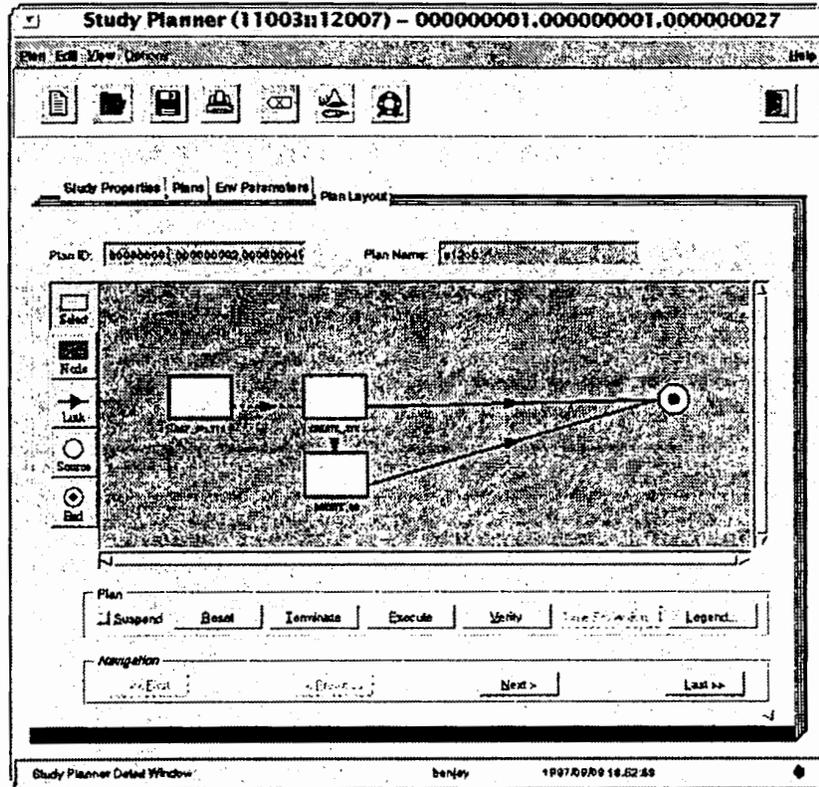


Figure 14. Use of environment variables to define stack criteria for major point sources.

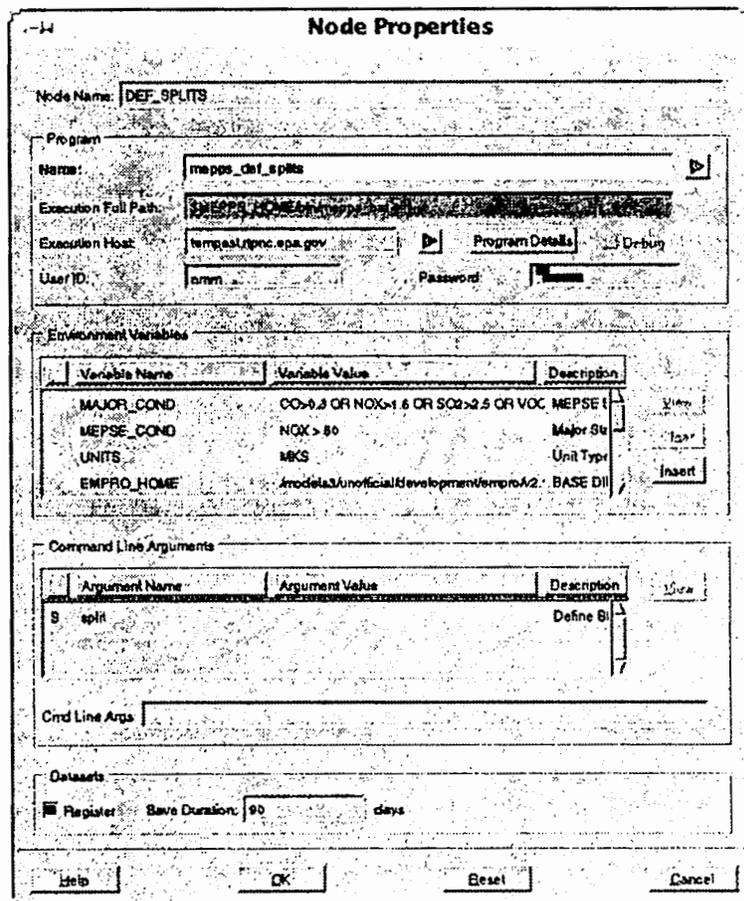


Figure 15. Use of environment variables in a Node Properties window to merge output files.

Node Properties

Node Name: CREATE_2D

Program

Name: mepps_create_2d

Execution Full Path: /usr/local/MEPPS/bin/mepps_create_2d

Execution Host: tempest.nrc.epa.gov

User ID: hnm Password: []

Program Details | Debug

Environment Variables

Variable Name	Variable Value	Description
AREA	YES	Include F
BIO	YES	Include E
LOGFILE	create2d.logfile	I/O API Lc
MOBILE	YES	Include h

View | Clear | Insert

Command Line Arguments

Argument Name	Argument Value	Description
S	spec2d	Create 2d

View

Cmd Line Args: []

Datasets

Register Save Duration: 90 days

Help | OK | Reset | Cancel

Figure 16. A typical listing of emission processing output files, including I/O API files, SAS® files (ssd01 suffix), and log files.

```

shelltool - /bin/csh
adayspec.ssd01      met.dat            run_desc.ssd01    spmvlc.ssd01
areaemis.ssd01     metadata.ssd01    spardrop.ssd01    spmvspec.ssd01
arsorprc.ssd01     mvofemis.ssd01   sparee.ssd01      spptdrop.ssd01
avptemis.ssd01     polid_species.dat sparlc.ssd01      spptee.dat
bioemis.ssd01      ptbase.dat        sparspec.ssd01    spptee.ssd01
debug.bi           ptbase.ssd01     spbidrop.ssd01    spptid.dat
emission.bi        ptemis.ssd01     spbiee.ssd01      spptlc.ssd01
episodes.dat       ptgroup.dat       spbilc.ssd01      spptspec.ssd01
episodes.ssd01     ptgroup.ssd01    spbispec.ssd01    spxxee.dat
error.bi           ptpoltot.ssd01   species.dat        spxxee.logfile
goppt.log          ptvars.ssd01     spemis_majg.ioapi spxxee.ioapi
gopxsp.log         qaplots.sct01    spemis_mepg.ioapi spxxid.dat
gridmvee.ssd01     report.bi         spemis_ming.ioapi stack_major.ioapi
hremis.bi          run_desc.in       spmvdrop.ssd01    stack_mepse.ioapi
log.bi             run_desc.met      spmvee.ssd01      stack_minor.ioapi
  
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TECHNICAL REPORT DATA

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16. ABSTRACT This paper presents a brief tutorial example and describes the benefits of emission inventory data processing for air quality using the windows of the Study Planner of the Models-3 environmental modeling system. The functions of the key windows and the procedure for using them are illustrated using a 21 column by 21 row spatial grid with 12 km cell resolution, centered on Birmingham, Alabama. The Study Planner makes manipulation of input data and processing programs relatively simple and flexible. Emission inventory processing that had often been accomplished step-by-step with large amounts of intensive labor, including quality control, spatial allocation (gridding), temporal allocation, and chemical speciation, has now been automated. It is not necessary to change processor coding for different study areas, spatial resolutions, and time, to remember the locations of data files and processors in the system, and to use command line instructions to initiate and control the processing for each step.		14. SPONSORING AGENCY CODE	
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