Implementation of the SMOKE Emission Data Processor and SMOKE Tool Input Data Processor in Models-3

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ABSTRACT

The U.S. Environmental Protection Agency has implemented Version 1.3 of SMOKE (Sparse Matrix Object Kernel Emission) processor for preparation of area, mobile, point, and biogenic sources emission data within Version 4.1 of the Models-3 air quality modeling framework. The SMOKE system includes MOBILE 5b to model on-road emissions and the Biogenic Emission Inventory System, Version 2 (BEIS 2) to model biogenic emissions. Although SMOKE may be operated from scripts outside of the Models-3 framework, integration within the system allows automatic registration and tracking of input and output files, as well as close coupling to the Community Multiscale Air Quality (CMAQ) modeling system and visualization tools by using the Net CDF I/O API data format convention. Models-3 also includes the SMOKE Tool to assist in preparation of emission input data for SMOKE. The SMOKE Tool performs basic functions for the user, including 1) import and quality checking of emission inventory and related data, 2) preparation of user-defined model grids and gridding of emission data and surrogates (SMOKE Tool requires a Geographic Information System (GIS), 3) preparation of user-defined "packet" files which instruct SMOKE to apply factors including growth, control, and reactivity analysis factors (individual species may be added or deleted by source and location), and 4) allows the user to edit input files. Manual preparation of input files outside of the system is possible, but increases the probability of human error and substantially increases the time needed for data preparation.

INTRODUCTION

The Models-3 air quality modeling framework was designed to be a flexible, multi-scale, multi-pollutant system, that would supercede the need to develop and maintain specialized regional air quality models for individual pollutants.[1] One purpose of the framework design was to ensure consistency of the data exchanged by traditionally separate modeling components (meteorology, emissions, and

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chemistry and transport), with regard to the spatial and temporal domains being used. This approach avoids many potential errors from use of inappropriate data, and allows easier tracking of input and output data files. Accordingly, the modeling of emission data was included as an integral component of the system. Modeling components that are fully integrated into the Models-3 system are capable of communicating at many levels with other modules of the system using the NetCDF (Common Data Format) I/O API (Input/Output Applications Programming Interface) format convention.

Emission Processor Development

When the Models-3 design effort began in 1992, there were no existing emission modeling and processing systems with the attributes necessary for full integration. The SMOKE was subsequently developed by the MCNC-North Carolina Supercomputing Center, Environmental Sciences Division, with U.S. EPA cooperation and support, for the purpose of being able to operate as a module within the Models-3 framework. The SMOKE is designed to be applicable to any air pollutant, and was originally applied to ozone precursor data in support of ozone modeling. The decision to develop and use SMOKE was based on an early recognition that the matrix computation paradigm in a Fortran program for modeling point, mobile, area, and biogenic emissions, is much faster than earlier sequential processing programs, i.e., one kind of operation at a time (area source processing, point source, etc.), that rely on SAS® software.[2]   This is true despite the fact that the current version of SMOKE, like its predecessor, the Models-3 Emission Processing and Projection System (MEPPS), uses Mobile 5b to model hourly mobile emission data[3], and the Biogenic Emission Inventory System, Version 2, to model hourly biogenic emission data[4]. For earlier releases of Models-3, a decision was made to modify an existing processor, the Geocoded Emission Modeling and Projection (GEMAP) system, for reasons of economy of resources and expediency.[5]   That system was the basis for the first Models-3 emission processor, MEPPS.[6] During 1998 and 1999, the SMOKE code was modified to fit directly within the Models-3 framework. The SMOKE had evolved since its inception and now provides additional features.[7] During 2000, SMOKE was made still more efficient, tested with additional pollutant species (including particulate emissions), tested within the current Models-3 framework design, and equipped with a module (Skmreport) for reporting and quality control.

Smoke Tool Functions

The SMOKE requires input in the form of emission data (often annual emission inventories) and related data which must be in acceptable formats, with files containing a defined spatial grid and spatial surrogates for area source emission data. Creation of these files is not trivial, and they cannot be created by SMOKE.   Therefore, SMOKE Tool was developed to provide these functionalities.   At this time SMOKE Tool is coded in the SAS© language, and has been configured to operate from the Models3 Study Planner and to provide input files in the required formats to SMOKE. Running from within Models-3, SMOKE Tool shares data with SMOKE and the Models-3 system by way of environment variables defined in the Models-3 Study Planner. Figure 1 presents an overview of the functional location of SMOKE and SMOKE Tool in the Models-3 system.

Using the Models-3 graphical interfaces, a user may define the horizontal and vertical grids of interest and episode (or case) in the Science Manager, and register data (including metadata) in the Dataset Manager. All of these items are then available to other system components, including SMOKE. This approach ensures consistency of basic information between the system components.

SMOKE

In order to use SMOKE in the Models-3 framework, it is necessary to use graphical

representations of a SMOKE "study" and "plans" (subsets of a study) in Study Planner's interactive interfaces. (Note: an emission study is a user-defined instance of a specific emission situation to be modeled.) Models-3 is provided with a typical SMOKE study (Figure 2), which is set for a tutorial, and several plans which address most anticipated uses of SMOKE (listed in Figure 3). This study can be copied and reused, or reannotated and reused by most users. Each study subset, or plan, is represented by an interactive graphical interface. Within a plan, individual algorithms or groups of algorithms, are represented by boxes (nodes), and linked by lines defining data dependencies. Plans have been constructed which include each core program defined in SMOKE on-line documentation.[8] The capabilities of the SMOKE core programs have been documented previously,[5] with exception of SMOKE Report (Smkreport). SMOKE Report is a post-processor to SMOKE which allows the user to specify many combinations of emission data for analysis and quality control purposes.

Figure 4 shows an example plan in which the SMOKE programs are graphically represented in the Models-3 Study Planner. This example shows the Skminven program, which imports emission inventories into SMOKE. Each plan and the nodes in it are annotated with environment variables which specify the logical names and physical locations of the needed inputs. Figure 5 shows the window listing the environment variables in the Smkinven plan. Given appropriate input data, a user need only re-annotate the logical or physical names of file locations in the links to fit a specific case of interest, and initiate and control program execution from the interface. Many names and locations will remain the same and annotations will not need to be changed. Each arrow which links nodes in a plan is annotated to give the location of the appropriate input and output files. Output files are automatically registered by the Models-3 Data Set Manager and placed in a standard output directory identified by the convention:
$M3DATA/studies/site_id/study_name/plan_name/run_number/node_name/
$M3DATA is an environment variable representing the location of the Models-3 data directory on a particular system. Site id is an identifier assigned to Models-3 system by EPA, and the study name is user defined. The plan and node names may be changed by the user, but there is usually little reason to do so because they are descriptive of the process included.

SMOKE TOOL

Because SMOKE requires input files in particular formats, the SMOKE Tool was created to assist the user in preparation of the files for emission modeling runs. The SMOKE Tool is in the SAS program language, and uses the Arc/Info geographic information system to create gridded files. The SMOKE Tool performs the following major functions:

- Creates a grid file for SMOKE, in accordance with the user-defined grid and projection definition taken from Models-3 Science Manager.
- Creates gridded ascii spatial surrogate files, using the grid file definition, which are used by SMOKE to apply the surrogates to emissions using spatial cross-reference files.
- Imports, checks and provides temporal and spatial cross-reference files (by source category code) for use in SMOKE.
- Allows import, editing, and modification of source specific chemical profile files, and grouping (lumping) to match the chemical mechanism being used in the air quality model in Models-3. Currently, the chemical mechanism lumping in SMOKE Tool supports the Carbon Bond 4 and RADM2 chemical mechanisms. The SMOKE will accept any species definitions, whether specific species or lumped species.
- Allows the user to specify the emission inventory files (and geographic subset thereof) to be used for a given emission modeling run.
- Allows the user to define "packets" of source category and geographically-specific factors for application in SMOKE to apply controls, future projections, adjustments, and reactivity

tests (changes in specific species).

The general procedure for using SMOKE Tool requires operation both from Models-3 Study Planner (first) and from the SMOKE Tool SAS windows (second) as follows:

1) It is necessary to first create the grid and spatial surrogate grid files to be used by SMOKE and SMOKE Tool. The grid definition must be established in the Models-3 Science Manager (see Figure 1). The nodes and links in the SMOKE Tool plan (Figure 6) must be annotated to refer to the grid name and to specify the spatial coverages to be used in generating the spatial surrogates by SMOKE Tool. Table 1 lists the environment variables used by the SMOKE Tool plan. Many of these variables are also used in SMOKE. The top node (grid_def) executes Arc/Info programs to create a grid file in accordance with the grid definition (referenced by environment variable HGRIDNAME). The second node (grid_cov) executes programs which grid the surrogate spatial coverages for the defined grid in accordance with the coverage definition file referenced by environment variable COVER_DEF. The final node of the plan (grid_srg) computes the spatial surrogates from the gridded data generated by the second node. Environment variable FEATURE_SRG references the surrogate feature table file containing a table of surrogate-specific features identifying the manner in which the surrogates will be computed. The coverage definition file and surrogate feature table file, along with a README_data_file, are located in the $M3DATA/nostudies/gisdb/ directory.

Table 1. Environment variables used by the Models-3 SMOKE Tool gridding plan.

Environment Variable	Example Value	Description
CENSUS_DATA	$M3DATA/nostudies /gisdb/census_block_ data	Census data. Contains housing and population data used to compute spatial surrogates in conjunction with the CENSUS GIS coverage.
EMS_HOME	$M3DATA/studies	Work space path
FEATURE_SRG	$M3DATA/nostudies /gisdb/feature_srg.in	Name of file containing the feature-surrogate table. Table defines the manner in which spatial surrogates are computed from GIS coverages.
HGRIDNAME	tut_36_c	Grid name (set when plan annotated with grid)
Coverage Name (example RAILROADS)	Y	Specifies whether a named GIS coverage is processed (Y for YES or N for NO - case insensitive). All spatial surrogates defined in the feature-surrogate table for the coverages selected will be generated. Eighteen surrogates are available for the U.S. and eleven for Canada.
COVER_DEF	$M3DATA/nostudies /gisdb/covdef.in	Name of file defining the GIS coverages available for the spatial surrogate calculation

2) Executing the SMOKE Tool plan generates ASCII format grid and gridded surrogate files for use by SMOKE and other portions of SMOKE Tool. Consequently, the SMOKE Tool plan must be run first. In order to create other input files required by SMOKE (emission inventories, cross-reference files, and packets), it is necessary to run SMOKE Tool through its interactive SAS windows.

3) The SMOKE Tool is accessed through the Models-3 Strategy Manager menu. The initial

SMOKE Tool window presents the choices Emission Mechanism, Emission Inventory, and SMOKE Input File. Emission Mechanism allows creation or editing of the species profiles and species lumping (grouping) consistent with the chemical mechanism selected within the Models-3 Community Air Quality Model (CMAQ). Normally, no changes to the mechanism grouping will be needed.

4) Next, within SMOKE Tool, the Emission Inventory selection is used to import, reformat, quality control, and export emission data (Figure 7). If a standard annual or other previously quality controlled inventory is being used, the user need only establish a working directory (using the Setup menu choice), define the geographic area (which may be done by referring to the grid using the menu option under Setup), and import the emission inventory files (usually point, area, and mobile source emission files) of interest using the import menu selection. Files are placed in Inventory Data Analyzer (IDA) format during export (export menu selection) before they are used with SMOKE. The IDA files are made available to the SMOKE input program (Smkinven) by annotating the graphical links in Smkinven plans. If emissions from more than one country are being used, they must be imported to separate user-defined subdirectories in the working directory, and then appended together on export (the user is prompted to append).

5) If the user wishes to define Major and/or Major Elevated (ie. sources for use with Plume in Grid modeling) points sources for SMOKE, the Stack Splits function in the Emission Inventory window of SMOKE Tool must be used to create two definition files (a group defnition and file and a stack definition file) for the SMOKE laypoint program.

6) Non-inventory files, such as spatial, temporal, and speciation cross-reference files needed by SMOKE are prepared in SMOKE Input File window of SMOKE Tool. SMOKE Input File requires the user to establish a working directory into which files are imported. Raw data are normally stored and imported from the $M3DATA/nostudies directory.   After import, the files may be quality controlled, edited and then exported. Importing converts files into SAS data sets. Quality control and editing are performed on the intermediate SAS data set files. Exporting places the files in the ASCII format required by SMOKE.

SMOKE also accepts files for projections and control of emissions in the form of packets in the file with logical name GCNTL (page 9-48 of SMOKE 1.3 draft User's Manual).[8] The packets consist of multiplicative factors in most cases. GCNTL subset files are:

- Adjustment packets allow user-defined modifications to emission inventory values by creating a file which applies percent factors by source category code and/or geographic area. Adjustment packets may also applied to emission inventories in the Emission Inventory section of SMOKE Tool.
- Allowable packets contain county, Standard Industrial Codes (SICs)(not yet supported in SMOKE), and Source Category Code (SCC)-specific controls, caps and replacement emission data.
- Control packets contain county and SCC-specific control levels for control efficiency, rule effectiveness, and rule penetration.
- CTG (Control Technology Guideline controls), such as Maximum Achievable Control technology (MACT) and Reasonably Available Control Technology (RACT)
- Projection packets use year, source-category-code, and geographically-specific percent factors (master tables are stored under $M3DATA/nostudies/projection/) to estimate future year emissions from a base year inventory, typically 1996.
- Reactivity packets (also user-defined) allow specification of individual chemical species (add, omit or replace) by source category and/or geographic area.

Packets are quality controlled, edited and prepared for export from SMOKE Input file using the Quality Control screen (Figure 9). Each packet is accessed, checked and edited as necessary, and then made available for export. The export function prepares the packet files for the SMOKE import (Smkinven) program, which accesses them by means of annotating a graphical link. packets, as described in the SMOKE Version 1.3 User Manual,[8] are given in Tables 2 and 3, respectively.

6) Finally, it is necessary to exit SMOKE Tool and Strategy Manager, and re-enter the SMOKE study and inventory input plan (Smkinven) in Models-3 Study Planner. The Smkinven input links (Figure 4) must be annotated by clicking on each of the graphical links and defining the physical location of the input files (click "view" under the logical name of each file).

Table 2. Control Packet Format.

Line	Columns	Description
1	A	/CONTROL/
2+	A	Country/State/County code (Integer)
	B	10-character SCC (Character)
	C	Pollutant ID (Character)
	D	Primary control equipment code (PCEC); -9 or 0 applies to all equipment (not yet supported in SMOKE)
	E	Control efficiency (1-100 %) (Real)
	F	Rule effectiveness (1-100 %) (Real)
	G	Rule penetration rate (1-100 %) (Real)
	H	Standard Industrial Category (SIC) (Integer) or -9 for missing
	I	Plant ID for point source (Character)
	J	Characteristic 1 (for IDA format, this is Point ID -9) (Character)
	K	Characteristic 2 (for IDA format, this is Stack ID or -9) (Character)
	L	Characteristic 3 (for IDA format, this is segment or -9) (Character)
	M	Characteristic 4 (blank for IDA format) (Character)
	N	Characteristic 5 (blank for IDA format) (Character)
3	A	/END/

Matching using PCEC or SIC is not yet supported. The valid key combinations are:

1) County, plant, Character (Char) 1, Char 2, Char 3, Char 4, Char 5, SCC, pollutant
2) County, plant, Char1, Char 2, Char 3, Char 4, Char 5, pollutant
3) County, plant, Char1, Char 2, Char 3, Char 4, pollutant
4) County, plant, Char1, Char 2, Char 3, pollutant

5) County, plant, Char1, Char2, pollutant
6) County, plant, Char1, pollutant
7) County, plant, pollutant
8) County, SCC, pollutant
9) Country/state, SCC, pollutant
10) County, pollutant
11) State, pollutant

Table 3. Projection Packet Format.

Line	Columns	Description
1	A	/PROJECTION *<4-digit **from** year><4-digit **to** year>*
2+	A	Country/State/County code or 0 (Integer)
	B	10-digit SCC, or left SCC with remaining digits filled in with zeros or 0 (Integer)
	C	Projection factor (Real)
	D	4-digit SIC, or 2-digit with remaining digits filled in with zeros or blank for missing (Integer)
3	A	/END/

The valid key combinations are:

1) Country, state, county, SCC
2) Country, state, SCC
3) Country, state, county
4) Country, state

EMISSION INPUT DATA

The Version 4.1 release of Models-3 with SMOKE 1.3 contains the most recent United States emission inventories and processing input files. In each case, users may add or substitute input files of their own. These input files are located in the Models-3 data structure as follows:

$M3DATA/nostudies/1km_landuse/
  /inventories/
  /gisdb/
  /packets/
  /projection/
  /smoke_tut/
      /ge_dat/
      /inventory/
      /met/
      /run_m3demo/
   /tigerdb/

where:
- $M3DATA is an environment variable representing the location of the Models-3 dataset directory.
- "1km_landuse" contains new 1km resolution gridded land cover for North America for use with the BEIS model in SMOKE.
- "inventories" contains annual national emission inventories including the revised 1990 NET inventory, 1995 revised NET inventory, and 1996 NET inventory (version 3.12), and an estimated 1995 Canadian inventory, all in IDA format. Other inventories may be added by users.
- "gisdb" contains the Geographic Information System (GIS) coverages used for creating emission spatial surrogate files. SMOKE Tool has been modified to allow users to add coverages and replace or modify a spatial surrogate cross-reference file.
- "packets" is the location of user-generated adjustment, control, projection, reactivity and related files used to adjust emissions (SMOKE logical file name GCNTL).
- "projection" contains the factor files used for future year projections by source category and geographic area through 2020, based on the recently updated Emission Growth and Analysis System, Version 4.[9]
- "smoke_tut" and its subdirectories contain specific pre-prepared input files needed for the tutorial study supplied with the Models-3 Version 4.1 release. Subdirectory ge_dat contains related general SMOKE input files such as spatial and temporal cross-references to source category codes.
- "tigerdb" contains optional coverages of roads for the United States based on the Tiger data base from the Bureau of the Census. These are not in the current spatial surrogate assignments.

The 1990 and 1995 inventories for the United States have been updated to include off road mobile emissions for sulfur dioxide and particulate matter. The 1996 United States inventory is the 1996 NET Version 3.12 inventory recently released. The emission inventory file formats are IDA. Temporal profiles, spatial surrogate coverages, and temporal and spatial cross-reference files are those developed by the U.S. EPA Office of Air Quality Planning and Standards for recent (late 2000 and 2001) modeling runs using SMOKE. One of the main changes for input data is the change from county level aggregate land cover (used by SMOKE to model biogenic emissions with Biogenic Emission Inventory System Version 2) to 1 km spatial resolution gridded land use data for North America. Coverages and principal features (with the names that need to be used in the system) used as spatial surrogates for the United States include:

- AGRICULTURE (US)
- AIRPORTS US
- AIRPORTS CANADA
- FHAROAD (US)
- LAND_WATER (US and CANADA)(separate features for land and island area)
- CENSUS (TOTHU as the feature for total housing units)
- CENSUS (TOTPOP as the feature for total population)
- ROADS (Major highways, urban primary roads)
- ROADS (Rural primary roads)
- PORTS (US and CANADA)
- RAILROADS (US and CANADA)
- LAND_WATER (Water area)

- • URBAN_RURAL (US and CANADA)(feature 1 urban areas, feature 2 rural areas)
- • FOREST (US and CANADA)
- • ROADS (US and CANADA) (feature 11 urban primary, roads12 rural primary, roads 21 urban secondary, 22 rural secondary)
- • CENSUS (URBPOP urban population)
- • CENSUS (RURPOP, rural population)
- • COUNTY (county area)

FUTURE PLANS

The next full release of the Models-3 air quality modeling framework will entail a completely new framework, as well as updates to the modeling components. We will replace the current framework, which is based on the C programming language, Object Store® database, Orbix® object communicator, and Galaxy® interface, with a Java-based framework being developed for the Multimedia Integrated Modeling System (MIMS). In fact, the Models-3 components other than the existing framework will become one of the initial portions (air medium) of MIMS. A description of MIMS may be found on the Internet at http://www.epa.gov/asmdnerl/mims/. Non-Java model components including SMOKE and CMAQ will be incorporated by the use of Java "wrappers" around them. We will replace the SMOKE Tool functions with other tools in the new framework, but not in time for the next Models-3 release. In the meantime, SMOKE Tool will remain available in its current form.

Near-term plans for SMOKE include incorporating the Mobile6[10] mobile source emission model to replace Mobile 5, and updating the Biogenic Emission Inventory System, Version 2, to Version 3. In addition, we will add the ability to define major and major elevated point sources within SMOKE (as opposed to within SMOKE Tool), and the ability to import and use Continuing Emission Monitoring (CEM) data from large point sources (usually electric utilities).

DISCLAIMER

The paper has been reviewed in accordance with the U.S. Environmental Protection Agency's peer and administrative review policies and approved for presentation and publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

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Figure 1. SMOKE and SMOKE Tool functions in Models-3.
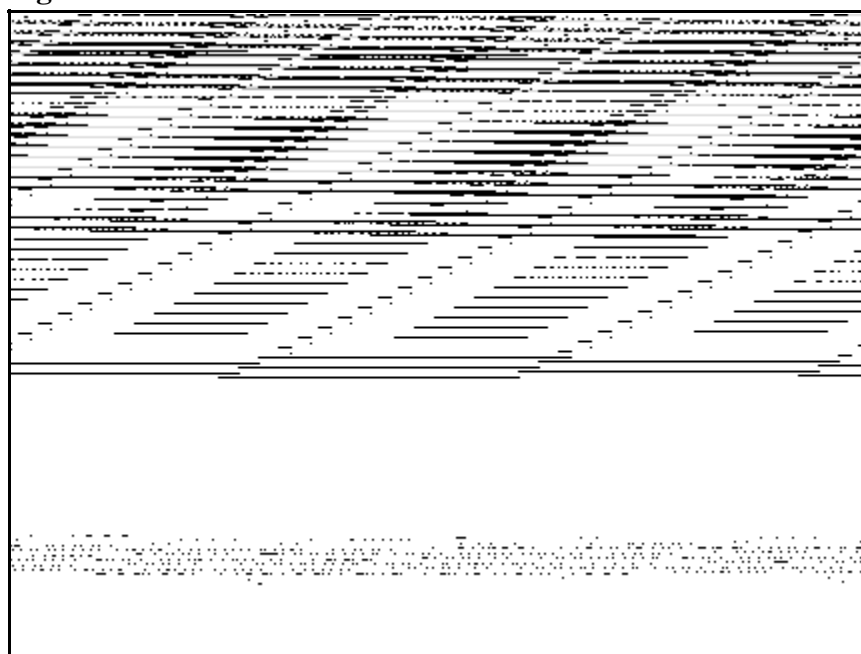
Figure 2. SMOKE study interface.

Figure 3. SMOKE plan listing

Figure 4. SMOKE inventory input plan.
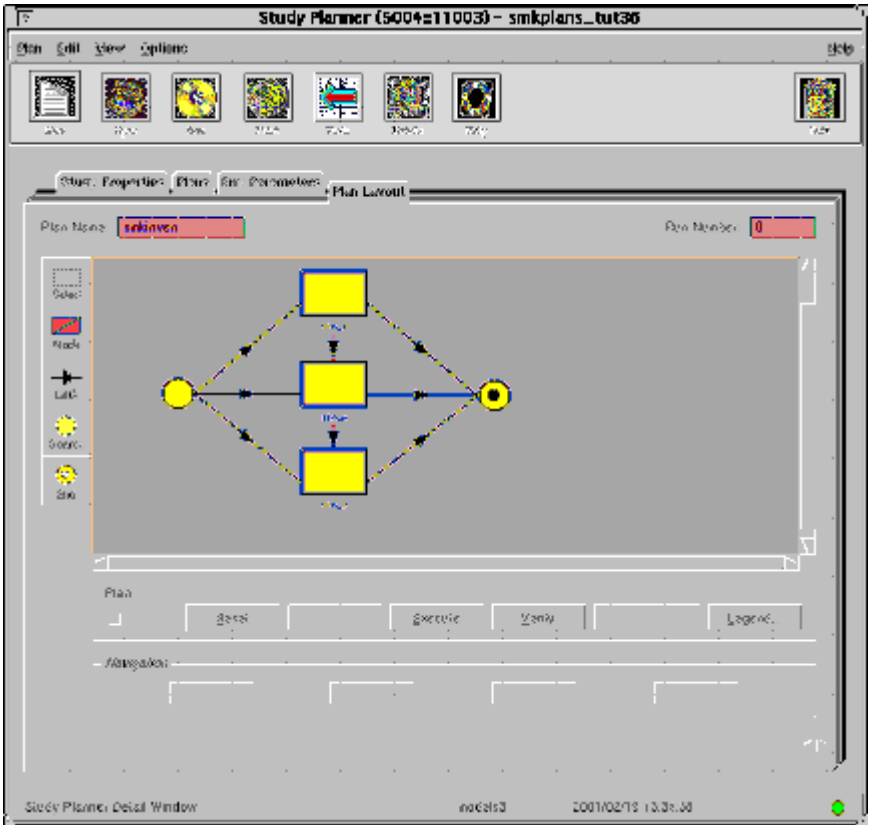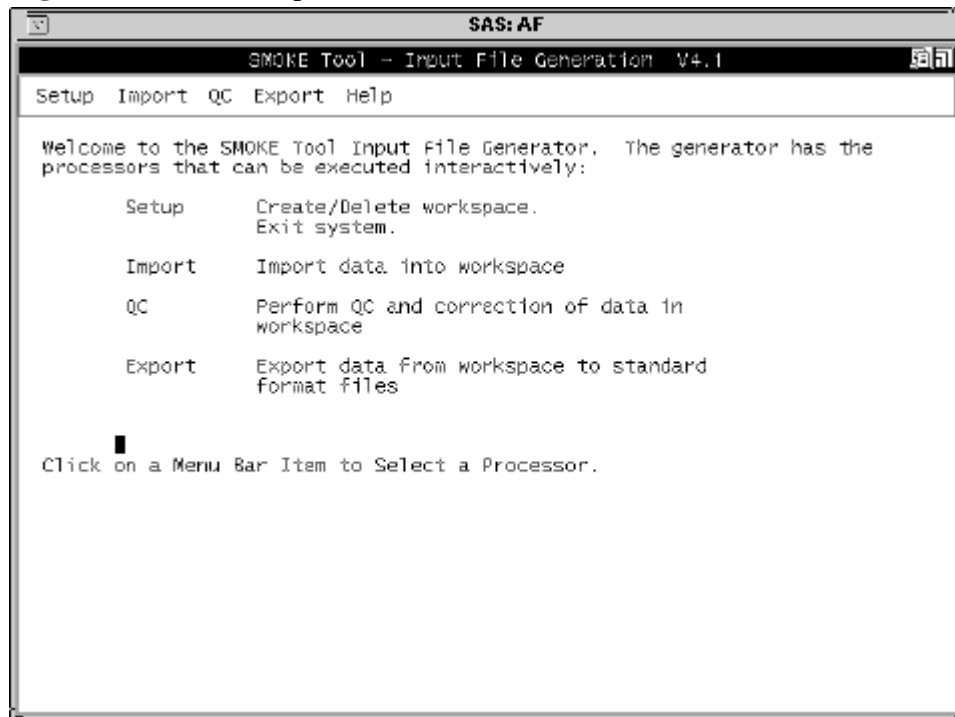

Figure 5. Environment variable screen

Figure 6. Models-3 SMOKE Tool gridding Study
Planner interface.
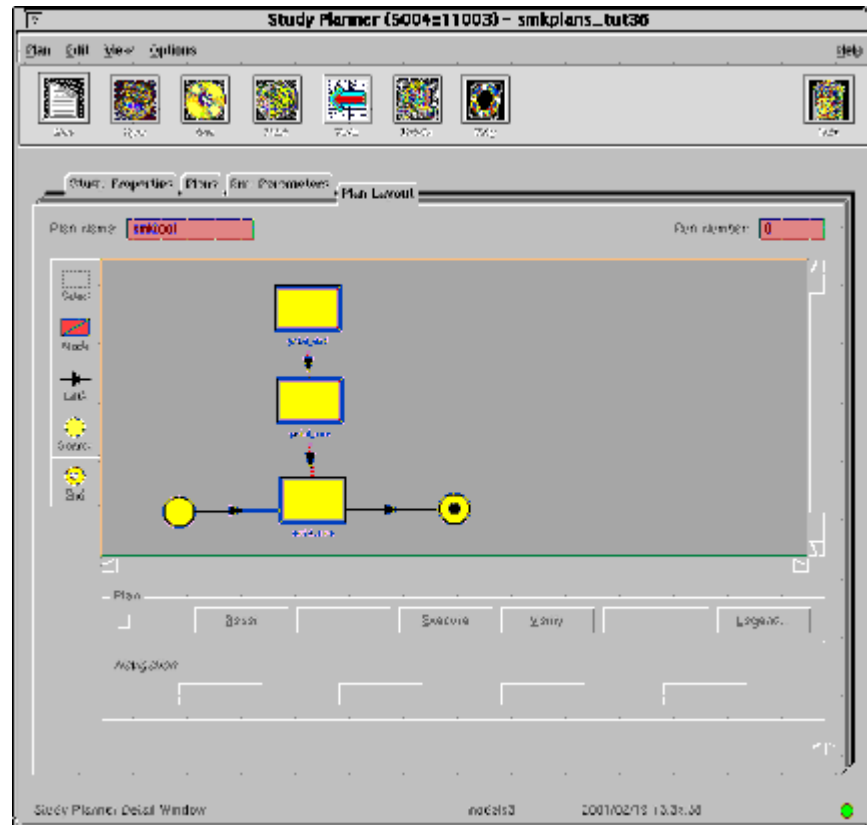
Figure 7. Emission Inventory window.
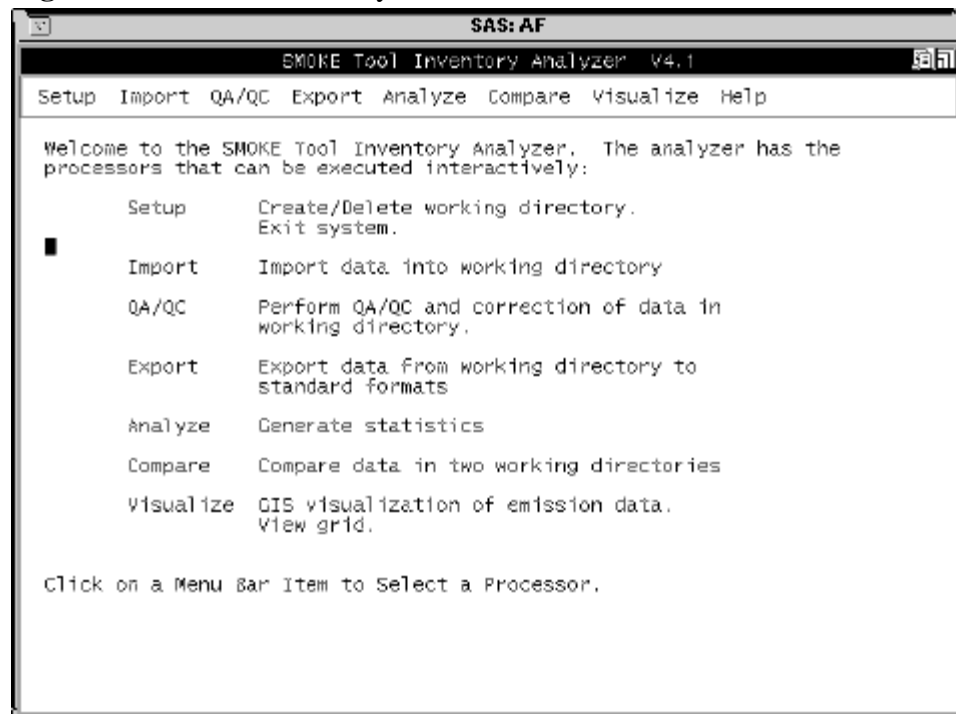
Figure 8. SMOKE Input File window.

Figure 9. Packet QC window.