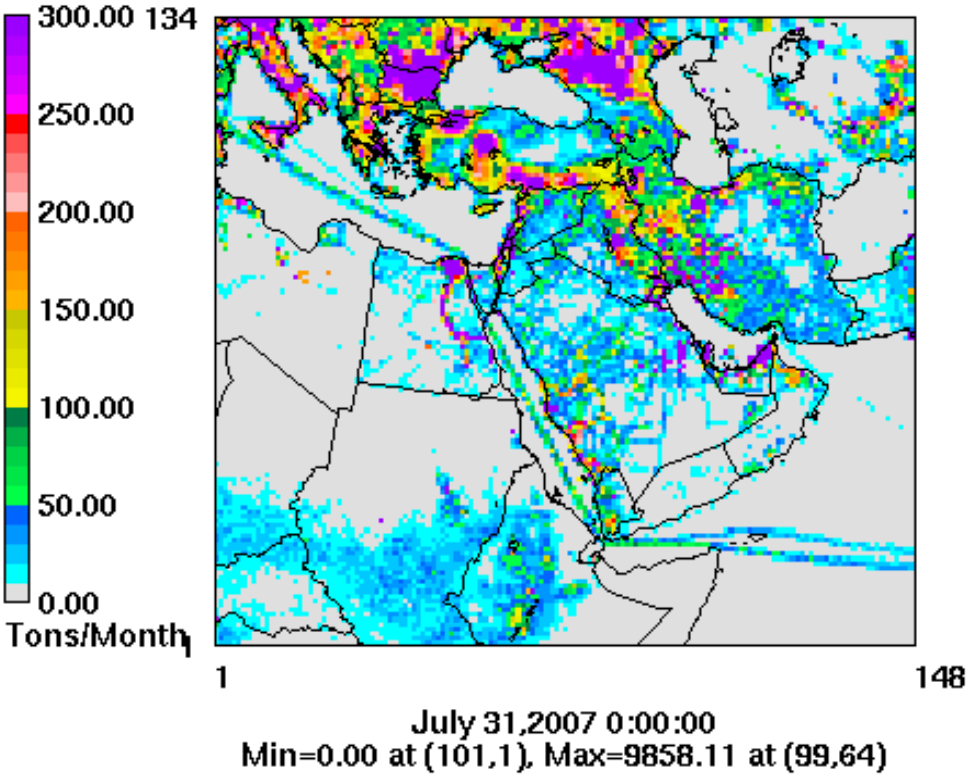
# Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System

## Monthly NO Emissions

## July 2007




## Introduction to SMOKE Version 3.1

## International Version

TRAINING MANUAL

Community Modeling and Analysis System Center

UNC Institute for the Environment

Chapel Hill, NC

## Disclaimer

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# ACRONYMS

| | |
|---|---|
| CAMx | Comprehensive Air Quality Model with eXtensions |
| CB-IV (or CB4) | Carbon Bond-IV chemical mechanism |
| CB05 | Carbon Bond '05 chemical mechanism |
| CEMPD | Center for Environmental Modeling for Policy Development (UNC-IE) |
| CMAS | Community Modeling and Analysis System |
| CMAQ | Community Multiscale Air Quality model |
| CTM | Chemical Transport Model |
| CVS | Concurrent Versions System |
| FIPS | Federal Information Processing Standards |
| GIS | Geographic Information System |
| GMT | Greenwich Mean Time |
| I/O API | Input/Output Applications Programming Interface |
| IDA | Inventory Data Analyzer |
| IE | Institute for the Environment (UNC) |
| MCIP | Meteorology-Chemistry Interface Processor |
| MM5 | Fifth Generation Mesoscale Model |
| NCAR | National Center for Atmospheric Research |
| NEI | National Emissions Inventory |
| NOAA | National Oceanic and Atmospheric Administration |
| $NO_x$ | Oxides of nitrogen |
| $O_3$ | Ozone |
| ORL | One Record per Line |
| PAVE | Package for Analysis and Visualization of Environmental data |
| PinG | Plume-in-Grid |
| PM | Particulate Matter |
| $PM_{2.5}$ | Particulate Matter less than 2.5 μm in diameter |
| PPB | Parts Per Billion |
| PPM | Parts Per Million or Piecewise-Parabolic Method advection scheme |
| PSU | Pennsylvania State University |
| SAPRC | State Air Pollution Research Center chemical mechanism |
| SCC | Source Classification Code |
| SMOKE | Sparse Matrix Operator Kernel Emissions processor |
| $SO_x$ | Oxides of Sulfur |
| UNC | University of North Carolina |
| UTC | Universal Time Coordinate |
| WRF | Weather Research and Forecasting model |

 

# COURSE AGENDA

**Day 1**

| | |
|---|---|
| 8:30 – 9:15 | Emissions processing basics |
| 9:15 – 10:00 | SMOKE basics |
| 10:00 – 10:15 | Break |
| 10:15 – 11:00 | SMOKE assigns file and scripts |
| 11:00 – 12:00 | Hands-on SMOKE overview |
| 12:00 – 1:00 | Lunch |
| 1:00 – 2:00 | Hands-on SMOKE overview (continued) |
| 2:00 – 3:15 | SMOKE programs and options |
| 3:15 – 3:30 | Break |
| 3:30 – 4:15 | SMOKE problem solving |
| 4:15 – 5:15 | Hands-on area-source processing |

**Day 2**

| | |
|---|---|
| 8:30 – 8:45 | Review |
| 8:45 – 9:45 | Hands-on area source processing (continued) |
| 9:45 – 10:30 | Hands-on biogenic processing with MEGAN |
| 10:30 – 10:45 | Break |
| 10:45 – 11:45 | Hands-on biogenic processing (continued) |
| 11:45 – 12:45 | Lunch |
| 12:45 – 3:00 | Hands-on point-source processing |
| 3:00 – 3:15 | Break |
| 3:15 – 5:15 | Hands-on gridded inventory processing |

**Day 3**

| | |
|---|---|
| 8:30 – 8:45 | Review |
| 8:45 – 10:15 | Hands-on merge processing |
| 10:15 – 10:30 | Break |
| 10:30 – 12:30 | Hands-on quality assurance |

# 1 SMOKE Training — Overview

## 1.1 Introduction

During this training overview, you will:

- Learn basic Linux commands needed for running SMOKE.
- Learn how to navigate around the main SMOKE directories.
- Learn how to use the Assigns file to set file and directory names needed by SMOKE.
- Explore the input and output directories.
- Review the locations of important SMOKE input files and see examples of them.
- Learn how to set up SMOKE for a new grid or episode.

The symbol ">" is used throughout the training materials to represent the Linux prompt. When this symbol appears as the first entry on a line in these instructions, you do not need to type it. Also, `Courier font` is used to indicate text that you should type at the prompt as you work through the exercises.

The login information for your training laptop is provided below. Keep this information handy for reference throughout the class.

**Login:** _____

**Password:** _____

## 1.2 Linux commands and information needed for training

1. The following is a brief tutorial of basic Linux commands needed for the SMOKE exercises.

> **NOTE:** In Linux the case is important (lowercase and uppercase are not interpreted the same way), so please follow the instructions carefully.

From the Main Menu (bottom left corner), open a terminal window by selecting Applications and then Accessories. There is also a Terminal icon on the toolbar.

A. Please read through the document titled "SMOKE Training – Linux Basics" if you have not already done so. It gives a quick overview of some important Linux concepts and also provides a list of most of the commands you will need for this class. In the next steps, we will try out some of the commands.

B. **Get a list of the contents of a directory.**
To list the contents of a directory, use the **ls** command, followed by the <Enter> key:

```
> ls
```

C. **Change directories.**
To change to a different directory, use the **cd** command. The syntax of this command is:

cd <directory name>

For example, to change to the subsys directory from your home directory, type the following command:

```
> cd smoke/subsys
```

To back out of a directory, type the following command:

```
> cd ../
```

To back out two directory levels, type the following command:

```
> cd ../../
```

D. **Use an environment variable.**
The following example uses the environment variable $SMKROOT to change to the root directory of the SMOKE system. To use an environment variable, the dollar sign must precede the environment variable with no space between the dollar sign and the environment variable. Type the following command to change to the SMOKE root directory (we will use capital letters for all environment variables):

```
> cd $SMK_HOME
```

**NOTE:** For the training, $SMK_HOME has been set for you in your environment. This will not be true for the SMOKE release case that you can download.

E. **Determine the value of an environment variable.**
The **echo** command permits you to see the value of an environment variable. For example, to see the value of the $SMK_HOME environment variable, type the following:

```
> echo $SMK_HOME
```

The contents of the variable will be displayed, and the Linux prompt will then return.

F. **Find out what directory you are currently in.**
The **pwd** command allows you to see the directory currently available at the Linux prompt. Depending on the configuration of your computer, this may also be displayed along with the Linux prompt. Type the following command to see your directory:

```
> pwd
```

 

G. **Copy a file.**
The **cp** command is used to make a copy of a file and give that copy a different name. The syntax of the copy command is:

cp <from filename> <to filename>

You will practice copying files when setting up for a new SMOKE run in step 4.

### *1.3 The SMOKE system directories*

2. The main SMOKE system directory is $SMK_HOME. From the xterm window, go to the main SMOKE system directory and look at its contents by typing:

```
> cd $SMK_HOME                    changes the directory
> ls                              shows directory contents
```

Several directory names will be displayed in your window:

- The **data** directory: location of all SMOKE input and output data
- The **scripts** directory: location of SMOKE administrative scripts
- The **subsys** directory: location of SMOKE system, libraries, and scripts

Change directories into the subsys/smoke directory and look at the contents by typing:

```
> cd subsys/smoke
> ls
```

Several directory names will be displayed in your window:

- The **assigns** directory: location for the Assigns files.
- The **doc** directory: location for the release notes for the current version of SMOKE.
- The **Linux2_x86_64pg** directory: location for the SMOKE programs.
- The **scripts** directory: location for the installation, compilation, and run scripts.

3. Go to the assigns directory and look at its contents by typing:

```
> cd assigns
> ls
```

Several file names will be displayed in your window:

- The file starting with "**ASSIGNS**" is the Assigns file.
- The **check_settings.scr** script is used by the Assigns file to ensure that various script settings are initialized.
- The **set_case.scr** script is used by the Assigns file to set the environment variables used in labeling directories and files for the case being run.
- The **set_dirs.scr** script sets input and output directory paths.

- The **setmerge_files.scr** script is used by the Assigns file to ensure that model-ready output logical file names are set, depending on the run script settings (e.g., if you are running the final merge step in SMOKE to get model-ready output files, this script will set the output logical file names).
- The **smk_mkdir** script is used by the Assigns file for creating input and output directories, and setting/checking write permissions.
- The **smk_rmfiles.scr** script is used by the Assigns file for deleting SMOKE intermediate and output files before each script run (only when AUTO_DELETE setting is set to Y).
- The **sysflags** script is called by the Assigns file to set up compiler and platform-specific environment variables.
- The **unset.scr** script unsets temporary environment variables used by the Assigns file.

## *1.4 Setting up for a new SMOKE run*

4. Now you will step through the various tasks needed for setting up for a new SMOKE simulation. Not all of these steps are required in all of the training exercises, but we will go through them all so that you are familiar with configuring SMOKE for new simulation.

   A. Create an Assigns file. The first step in using a new inventory, episode, grid, or emissions scenario is creating a new Assigns file. You will copy the Assigns file in the **assigns** directory to a new file that uses your initials in its name.

   > **NOTE:** With Linux, you can use the tab key to automatically complete file names. If you start typing a file name at the prompt and then press the tab key, the computer will try to fill in the rest of the file name for you. Try this in the next command.

   Type the following at the prompt:

   ```
   > cp ASSIGNS.mideast07.cmaq5.cb05p25.uae36
   ASSIGNS.train_<initials>.cmaq5.cb05p25.uae36
   ```

   For example, if your initials are AB:

   ```
   > cp ASSIGNS.mideast07.cmaq5.cb05p25.uae36
   ASSIGNS.train_ab.cmaq5.cb05p25.uae36
   ```

   Typically, you will copy a previously created Assigns file to a name that corresponds to the new emissions scenario. Here, we are using the emissions scenario name "train_<initials>".

   The abbreviation "uae36" in the Assigns file name is the grid name and indicates a 36-km grid centered in Abu Dhabi, United Arab Emirates. As you will see, this grid name is used in naming the SMOKE input and output files.

   B. Edit the Assigns file you just created. In this documentation, we will use an editor called **gedit**, but you can use any Linux text editor you like (that is available on your computer).

 

**NOTE:** The ampersand ("&") at the end of the command runs the editor in the background so that you can continue the training. Remember that you can use the tab key to complete file names.

```
> gedit ASSIGNS.train_<initials>.cmaq5.cb05p25.uae36 &
```

In this file, change the values of the following environment variables as indicated:

- ☐ Change the value of INVOP (base year inventory output name) to train_<initials>.
- ☐ Change the value of INVEN (base year inventory output name with version) to train_<initials>.
- ☐ When you change INVOP, any environment variables that are based on $INVOP change as well.

**Exercise 1-1:**
What is the first environment variable in the file whose value will change because you changed INVOP?

**Answer 1-1:**

Save the file.

C. To make sure the Assigns file works correctly, and to create the input and output directories for your new inventory and scenario, source the Assigns file by typing the following:

```
> source ASSIGNS.train_<initials>.cmaq5.cb05p25.uae36
```

The Assigns file will print out some information about the system you are working on and then return the Linux prompt.

D. To see all of the environment variables that are now available for running SMOKE, type the command:

```
> env | more
```

**NOTE:** The "|" or "pipe" symbol is above the "Enter" key on your keyboard. In Linux, this symbol is used to string commands together. Here, we are causing the output from the env command to scroll by with the more command.

Scroll through the list by pressing the space bar on the keyboard. The first environment variable that has been set by the Assigns file is INVID. You can quit **more** by typing "q".

E. The Assigns file also created output directories, such as $INVOPD, $STATIC, $SCENARIO, $OUTPUT, and $REPSCEN. You can confirm this by using the **cd** command to change to some of these directories. For example:

```
> cd $STATIC
> ls
```

F. The final step in setting up for a new run is creating the input files. The steps in the next section will help you become more familiar with the input directories and files.

## *1.5 Input and output directories and input files*

Once you have invoked the Assigns file, you can directly access many directories using environment variables.

5. Review the primary input directories and their files in $INVDIR and $GE_DAT.

A. Go to the inventory input directory and look at the contents of the directory:

```
> cd $INVDIR
> ls
```

B. Within the $INVDIR directory are the area, biog, gridded, mobile, nonroad, point, and other directories, where the raw emissions, land use data, and Smkreport configuration files are stored. These directories correspond to the $ARDAT, $BGDAT, $GDDAT, $MBDAT, $NRDAT, and $PTDAT environment variables set by the Assigns file.

C. Look in these directories and view some the inventory files that are there. Note that the mobile and nonroad directories are empty. Below is a sample of the input inventory logical file names and their physical file counterparts as set in the Assigns file.

| | | |
|---|---|---|
| **ARINV:** | area/arinv.ar.lst | area-source inventory file |
| **ARINV:** | area/arinv.areng.lst | industrial area-source inventory file |
| **PTINV:** | point/ptinv.lst | point-source inventory file |

D. The arinv.ar.lst, arinv.areng.lst, and ptinv.lst files are list files that contain the file names of actual raw inventory files; for this training, we are using both IDA and ORL-formatted raw inventory files. The area-source inventory (ar) lists two raw inventory files, while the area/energy sector inventory (areng) and point-source inventories list only one raw inventory file each. You can use list files to combine as many raw inventory files as you need.

You may also set the input logical file names (e.g., ARINV) to an ORL or IDA-formatted file directly, if you have only a single file to input. These variables can be changed in the Assigns file.

E. Change directories to the area inventory directory and view the area-source inventory files, **arinv_mideast05.orl** and **aginv_mideast05.ida,** using the **more** command, for a discussion about these files with the instructor:

 

```
> cd $ARDAT
> more arinv_mideast05.orl
> more aginv_mideast05.ida
```

F. View the point-source inventory file **ptinv_abudhabi04.orl** using **more**, for a discussion about this file with the instructor:

```
> cd $PTDAT
> more ptinv_abudhabi04.orl
```

G. Go to the "other" directory and examine that directory's contents:

```
> cd $INVDIR/other
> ls
```

The $INVDIR/other directory contains:

- ☐ The inventory table (invtable.txt)
- ☐ The report configuration files used by Smkreport (repconfig*)
- ☐ The area-to-point assignments file used by **Smkinven** (artopnt.1999.txt)

H. Open the inventory table that we are using for this training using **gedit**, for a discussion about this file with the instructor:

```
> gedit invtable.txt &
```

I. Go to the general data (GE_DAT) directory and look at that directory's contents:

```
> cd $GE_DAT
> ls
```

The $GE_DAT directory contains files that are shared by all source categories, such as cross-reference files, gridding surrogates, and temporal and speciation profiles.

**Exercise 1-2:**
What is the name, including the directory path, of the speciation profile file? (*Hint:* Look in Chapter 8 of the SMOKE User's Manual to find the logical file name of the speciation profile file, then look in the Assigns file for that logical file name.)

**Answer 1-2:**

J. As a group, we will look at the contents of the following files using **gedit**:

| | |
|---|---|
| **AGPRO, BGPRO, MGPRO:** | UAE36/WORLD_1_NOFILL.txt<br>UAE12/WORLD_1_NOFILL.txt<br>(gridding surrogates) |

| | |
|---|---|
| **AGREF, MGREF:** | amgref.mideast.txt<br>(gridding cross-references) |
| **ATPRO, MTPRO, PTPRO:** | amptpro.mideast.txt<br>tpro_bioburn.txt<br>(temporal profiles) |
| **ATREF, MTREF, PTREF:** | amptref.mideast.txt<br>tref_bioburn.txt<br>(temporal cross-references) |
| **GSPRO:** | gspro.cmaq5.cb05p25.txt<br>gspro_bioburn.txt<br>(speciation profiles for CMAQ) |
| **GSREF:** | gsref.cmaq5.cb05p25.txt<br>gsref_bioburn.txt<br>(speciation cross-reference) |
| **GSCNV:** | gscnv.txt<br>gscnv_cb05.bioburn.txt<br>(pollutant-to-pollutant conversion file) |
| **LAYER_FRACTION:** | layers_gfed.txt<br>layers_areng.txt<br>(layer allocation fractions) |

6. There are also files that are used by all source categories that are not cross-reference files, profiles, or surrogates. Look at each of the following files with the instructor.

   In the general data directory:

| | |
|---|---|
| **GRIDDESC:** | GRIDDESC<br>(grid descriptions file) |
| **COSTCY:** | costcy.txt<br>(country, state, and county file) |
| **HOLIDAYS:** | holidays.txt<br>(list of holiday dates and the day of the week to use for setting day-of-week and diurnal temporal profiles) |
| **PROCDATES:** | procdates.txt<br>(time periods to be processed by **Temporal**) |
| **SRGDESC:** | $GE_DAT/UAE36/SRGDESC.txt<br>$GE_DAT/UAE12/SRGDESC.txt<br>(the codes, descriptions, and location of the surrogate files) |

 

**SCCDESC:** scc_desc.txt
(the source category code descriptions)

**SICDESC:** sic_desc.txt
(the standard industrial classification [SIC] code descriptions)

7. Take a look at each of the primary intermediate and final output directories $SCENARIO, $STATIC, $OUTPUT, $REPSCEN, and $REPSTAT. Note how the value of the $EBASE variable (i.e., train_<initials>) is used in these paths.

**Exercise 1-3:**
What environment variable is common to the values of the output directory environment variables listed above? (*Hint:* Use the set_dirs.scr script in the Assigns directory to determine this.)

**Answer 1-3:**

## *1.6 Setting up for a new grid*

8. Now you will step through the various tasks needed for setting up a new grid. In this case, we will set up an 8-km grid that also focuses on Nashville, Tennessee, USA.

   A. Copy your Assigns file to a file with a different grid name as the final part of the file name:

   ```
   > cd $ASSIGNS
   > cp ASSIGNS.train_<initials>.cmaq5.cb05p25.uae36
   ASSIGNS.train_<initials>.cmaq5.cb05p25.uae12
   ```

   B. Use **gedit** to edit the 12-km Assigns file. Change the GRID environment variable value to the grid name "UAE12".

   C. The IOAPI_GRIDNAME_1 variable sets the name of the grid definition as defined in the $GE_DAT/GRIDDESC file. For these training exercises, the 12-km grid information is already entered in the GRIDDESC file with the name UAE12LCC_78X72. Change the IOAPI_GRIDNAME_1 variable to this value.

   When setting up new grids in SMOKE, you will need to point the Assigns file to a GRIDDESC file that contains the definition for the new grid, and set the IOAPI_GRIDNAME_1 variable to the name of the grid listed in the GRIDDESC file.

   D. Change the meteorology scenario name (METSCEN) to UAE_MCIP12.

E. Change the SRGDESC and SRGPRO_PATH settings to the directories containing the 12-km spatial surrogates: $GE_DAT/UAE12/SRGDESC.txt and $GE_DAT/UAE12/, respectively.

Save the Assigns file.

### 1.7 Setting up for a new episode

9. To set up for new dates, you must change the following variables in the Assigns file:

- EPI_STDATE: The episode start date in Julian date format (YYYYDDD)
- EPI_STTIME: The episode start time (HHMMSS)
- EPI_RUNLEN: The episode run length (HHMMSS)
- EPI_NDAY The number of days in the episode
- G_STDATE: The start date in Julian (YYYYDDD) for the model-ready output files.
- G_STTIME: The start time (HHMMSS) for the model-ready output files.
- G_RUNLEN: The length (HHMMSS) of each model-ready output file.
- ESDATE: The start date (YYYYMMDD) used in file names.
- NDAYS: The number of days in each model-ready output file.

The SMOKE scripts will loop through the number of days indicated by EPI_NDAY, incrementing G_STDATE and creating the model-ready output files for each day. During each loop, the ESDATE variable is also updated and is used for naming output files.

A. Look at the Assigns file using **gedit** to see where these variables are in the file. Note that the G_TSTEP variable is also in the file, but its value will not change SMOKE's output. SMOKE can output only hourly data.

**Exercise 1-4:**
What are the values of the environment variables listed below?

**Answer 1-4:**

EPI_STDATE:

EPI_STTIME:

EPI_RUNLEN:

EPI_NDAY:

G_STDATE:

G_STTIME:

G_RUNLEN:

ESDATE:

NDAYS:

 

You do not need to do anything in this step except review the script settings.

B. Confirm that the Julian and Gregorian starting dates are consistent. The I/O API program **juldate** will convert a Gregorian date to a Julian date, and has the following syntax:

juldate <month> <day> <4-digit year>

For example, to determine the Julian date for April 21, 2004:

```
> juldate 4 21 2004
```

This completes the SMOKE Overview exercise. You are now ready to move on to the second exercise, which addresses area sources.

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# 2 SMOKE Training — Area Sources

## 2.1 Introduction

During this area-sources training, you will:

- Copy the area-sources run script, examine the script, and change options.
- Process 2-d and 3-d area-source emissions for the CMAQ model.
- Examine area-source program logs and reports.
- Examine area-source emissions files in PAVE.
- Problem solve for processing area sources on a new grid.

The symbol ">" is used throughout the training materials to represent the Linux prompt. When this symbol appears as the first entry on a line in these instructions, you do not need to type it. Also, `Courier font` is used to indicate text that you should type at the prompt as you work through the exercises.

**NOTE:** To proceed with this lab, you must have created an Assigns file for the uae36 grid, as described in the SMOKE Overview Exercise. Use the following command to source your Assigns file:

```
> source $SMKROOT/assigns/ASSIGNS.train_<initials>.cmaq5.cb05p25.uae36
```

## 2.2 The run script and script options

1. In this step, you will copy the area-sources run script and configure it to use your Assigns file and to run SMOKE for inventory import, gridding, and merge. The following steps will guide you through this process.

   A. Go to the directory that contains the SMOKE run scripts:

   ```
   > cd $SCRIPTS/run
   ```

   B. Copy the area-sources script to one that uses your initials. In the instructions below, fill in your initials where indicated, as you did for the Assigns file. Remember that you can use the tab key to complete file names.

   ```
   > cp smk_ar_mideast07.csh smk_ar_train_<initials>.csh
   ```

   C. View your area-sources script using the following command:

   ```
   > gedit smk_ar_train_<initials>.csh &
   ```

   D. Examine the script. Note that at the top of the script the SMK_SOURCE environment variable is set to "A", indicating that area sources should be processed. Below that, the script sets which programs to run using the RUN_* variables. Next, the program-specific

and then the multiple-program environment variables are listed. These variables control individual program behavior and the behavior of two or more programs, respectively. Finally, the Assigns file is sourced and the programs are run.

E. Change the Assigns file name to use the Assigns file that you created for the uae36 grid in the Overview lab.

F. Change the appropriate RUN_* environment variables to configure the script to run the programs for:

- ☐ Run the inventory import program (Smkinven)
- ☐ Run the gridding program (Grdmat)
- ☐ Run the merge program (Smkmerge)

**Exercise 2-1:**
What were the names of the RUN_* environment variables that were set to Y?

**Answer 2-1:**

1. 2. 3.

Find the section of the script that controls the Smkmerge program. Change the following settings for Smkmerge:

- ☐ Output a gridded file, state totals, and county totals
- ☐ Output the gridded emissions and the state and county totals in tons/day
- ☐ Do not produce temporally allocated output
- ☐ Do not produce speciated output

**Exercise 2-2:**
List the environment variables that you changed or checked the values of.

**Answer 2-2:**

1. 2. 3.

4. 5. 6.

7.

G. Save the run script.

 

## 2.3 Running the area-sources inventory import, gridding, and intermediate merge

2. In this step you will import the area-sources inventory, create the gridding matrix, and merge the results to create a gridded inventory. The gridded inventory merge is not an essential step for creating model-ready input files (which need to be hourly and have chemical speciation). However, the intermediate merge step can be used as a quality assurance step, and we will use it as part of the learning process.

   A. Run the area-sources run script:

      ```
      > smk_ar_train_<initials>.csh
      ```

   B. While the script is running, various messages from each of the programs will scroll by on the screen. This same information is written to the log file for each program.

   C. If you need to rerun a program, the run script is set up to create backup copies of existing log files rather than deleting them. The setting AUTO_DELETE_LOG in the "Script Settings" section of the run script controls whether old logs are deleted or renamed. For the training, you will save your old log files so that you or the instructor can look back at previous log files.

## 2.4 Examine the log files and output files

3. An important part of running SMOKE is examining the log files for notes, warnings, and errors. For notes and warnings, you must decide whether they indicate problems or can be ignored. If there are errors, you must fix them because the programs will not complete successfully if an error occurs. We will examine the log files and also look at the gridded inventory and state and county totals.

   A. Go to the directory containing the log files for area sources:

      ```
      > cd $LOGS
      ```

   B. Confirm that all programs completed successfully. When a SMOKE program completes successfully, it will write the following message to the log file:

      ```
      --->>  Normal Completion of program <PROGRAM NAME>
      ```

      You can check the end of a log file using the **tail** command:

      ```
      > tail smkinven.ar.train_<initials>.log
      ```

      Use this command to make sure that all of your log files end with the "Normal Completion" message.

   C. View the log file for **Smkinven** using **gedit**:

      ```
      > gedit smkinven.ar.train_<initials>.log &
      ```

**Exercise 2-3:**
What are the five major types of warnings that appear in this log file?

***Tip**:* You can use the Linux command **grep** to find words in a text file. For example, the following command will find all instances of the word WARNING in the **Smkinven** log file and then sort the unique lines:

```
> grep WARNING smkinven.ar.train_<initials>.log | sort –u
```

**Answer 2-3:**

1.

2.

3.

4.

5.

D. Exit from the gedit window.

E. Now go to the inventory output directory to examine the output files from **Smkinven**:

```
> cd $INVOPD
> less asrc.ar.txt      (use the space bar to scroll and the "q" key to quit)
> less area.map.ar.train_<initials>.txt
> ncdump area.ar.ncf | less
```

**NOTE: ncdump is a netCDF utility that allows you to view binary netCDF files as text. While in ncdump, you can scroll forward with the <space bar>, backward with <b>, and use <q> to quit.**

**Exercise 2-4:**
What is the setting for the number of rows in the header of the area.ncf file? What does this correspond to in terms of the area-source inventory? *Hint:* Look in Chapter 9 of the SMOKE User's Manual for descriptions of the **Smkinven** output files.

**Answer 2-4:**

F. You can also convert the NetCDF file to a text file with the following command:

```
> ncdump area.ar.ncf > area.ar.out.txt
```

 

G. Now go to the reports directory to examine the gridded inventory report:

```
> cd $REPSTAT
> ls
> gedit repag.ar.UAE36.train_<initials>.rpt
```

You can compare your report file with the answers in the $ANSWERS/area/step_2/ directory.

> ***Tip**:* You can use the Linux command **diff** to compare two text files. The syntax of the command is as follows:
>
> diff <first file> <second file>

Exit from the text editor.

H. Start PAVE so you can use it to look at the gridded inventory file. **NOTE: If you are unfamiliar with PAVE, you may need assistance from the instructor(s) after starting PAVE.**

```
> pave –f $REPSTAT/ag.UAE36.train_<initials>.ncf
```

The gridded inventory file (**ag.UAE36. train_<initials>.ncf**) is in the $REPSTAT directory. The file can be added to the PAVE session using the command line argument "-f <directory/filename>, as shown above or by using the PAVE "Add/Delect/Select Dataset popup" window. To use the "Add/Delete/Select Datasets_popup" window, select the "Add" button in this window to load the gridded inventory file into PAVE.

Click a variable in the Species List under to select a variable for plotting. Highlight the variable that you would like to plot in the "Add/Delete/Select Formula_popup" window. The from the Graphics pull down menu in the main PAVE window select "Create Tile Plot".

Create a second tile plot with the gridded inventory file in the $ANSWERS/area/step_2/ directory. Compare this with the tile plot of your file to make sure you have processed the area sources correctly.

Continue to experiment and explore with PAVE. You may want to lower the maximum value in the map legend using the plot "Configure" menu. From the Control pull down menu in the plot window select "Configure" and "Tile". Enter a new number in the Max legend range box and hit <enter>. For example, plot CO emissions and change the maximum scale to 50. Also, try different formulas/species, and zoom functions within PAVE.

Exit from PAVE when you are finished.

## 2.5 Running the area-sources speciation, temporal allocation, and merge

4. In this step, you will configure the run script to run area-source speciation, temporal allocation, and merge. Then you will run the modified script. Note that we could have run all of these steps during the previous exercise, but by running these steps incrementally we're demonstrating the modularity of SMOKE. In this exercise we will not need to rerun the inventory import and gridding steps because they were successfully completed in the previous exercise.

   A. Navigate back to the run scripts directory.

   ```
   > cd $SCRIPTS/run
   ```

   B. Edit the **smk_ar_train_<initials>.csh** script to:

   - ☐ Run the speciation program (Spcmat)
   - ☐ Run the temporal allocation program (Temporal)
   - ☐ Run the merge program (Smkmerge)
   - ☐ Do not run the inventory import (Smkinven) or gridding programs (Grdmat)
   - ☐ Configure Smkmerge to produce temporally allocated and speciated output
   - ☐ Configure Smkmerge to output gridded emissions in moles/s (the units needed for CMAQ modeling)
   - ☐ Configure Smkmerge to output state totals in moles/hr
   - ☐ Do not output county totals

   C. Execute the area-sources script from the $SCRIPTS/run directory.

   After the programs have finished, confirm that all of the programs completed successfully using the **tail** command on the log files in the $LOGS directory. You can compare your log files and the $REPAGTS_L file (**repagts_l.ar.20070601.1.UAE36.train_<initials>.rpt** in the $REPSCEN directory) to the answers in $ANSWERS/area/step_4/.

## 2.6 Processing 3-d area sources

5. Emission inventories for sources that are emitted from elevated stacks, such power plants and smelters, or sources that have a vertical distribution due to the physical nature of the emission process, such as biomass burning and airport landing-take off cycles, require data about emissions heights in order to correctly represent these sources in air quality modeling systems. Emissions data are most commonly distributed as area source inventories, which do not inherently contain sufficient information to allocate the emissions to vertical model layers. Published or a priori information can be used to develop vertical profiles for generating vertically-resolved area source emissions for input to air quality modeling systems. In this step, you will process an area source inventory of energy sector sources, which consists primarily of power generation and petroleum refining facilities. The processing sequence is exactly the same as the previous step except for a final post-merge

 

step to allocate the emissions to the vertical model layers using information published in the literature for the energy sector. The SMOKE utility **Layalloc** will be used in this exercise to convert the 2-d energy sector area source emissions to 3-d emissions files.

A. Return to the $SCRIPTS/run directory, copy the area source run script used in the previous exercise to a new file named smk_areng_train_<initials>.csh, and open this script in a text editor:

```
> cd $SCRIPTS/run
> cp smk_ar_train_<initials>.csh smk_areng_train_<initials>.csh
> gedit smk_areng_train_za.csh &
```

B. Configure the script to import the area energy sector inventory, grid, speciate, temporalize, and merge.

- ☐ Change the SRCABBR environment variable to areng
- ☐ Run the inventory import program (Smkinven)
- ☐ Run the speciation program (Spcmat)
- ☐ Run the gridding program (Grdmat)
- ☐ Run the temporal allocation program (Temporal)
- ☐ Run the merge program (Smkmerge)
- ☐ Configure Smkmerge to output temporally allocated and speciated emissions
- ☐ Configure Smkmerge to output gridded emissions in moles/s
- ☐ Do not output state totals
- ☐ Output county totals with units of moles/yr

Save the run script.

C. Run the energy area-sources script from the $SCRIPTS/run directory:

```
> smk_areng_train_<initials>.csh
```

After the programs have finished, confirm that all of the programs completed successfully using the **tail** command on the log files in the $LOGS directory. You can compare your log files to the answers in $ANSWERS/area/step_5/.

6. Now open the energy sector area-sources run script and configure it to run the 2-d layer allocation program.

- ☐ Do not run the inventory import program (Smkinven)
- ☐ Do not run the speciation program (Spcmat)
- ☐ Do not run the gridding program (Grdmat)
- ☐ Do not run the temporal allocation program (Temporal)
- ☐ Do not run the merge program (Smkmerge)
- ☐ Run the 2-d layer allocation program (Layalloc)

Save and exit from the energy sector area-sources run script.

A. Examine the **Layalloc** input file in the $GE_DAT directory. Use a text editor to view the file **layers_areng.txt**. This file contains four, comma-separated columns in each row. The rows in this file correspond to different emission altitude bands. The first column represents the emission altitude band number, this is not related to the meteorology layers. The second and third columns contain the bottom and top emission heights, respectively, in meters from the surface for each emission layer. The fourth column is the fraction of emissions to allocate to each emission layer. The file **layers_areng.txt** specifies that there will be zero emissions up to 184 meters from the surface, 8% of the emissions will be between 184 and 324 meters, 46% of the emissions between 324 and 522 meters, etc.

   The program **Layalloc** maps the emission heights in meters contained in the layers file to the layers defined by the input meteorology data to produce vertically-resolved emissions using a sigma-p coordinate. **Layalloc** requires a METCRO3D file as an input to define the vertical layer structure.

B. Run the energy sector area-sources script from the $SCRIPTS/run directory:

```
> smk_areng_train_<initials>.csh
```

   Look for the following to confirm that Layalloc completed.

```
--->>  Normal Completion of program LAYALLOC
```

## 2.7 Examine the final model-ready files

Start PAVE:

```
> PAVE
```

Load the $AGTS_L files from the step 5 and step 6 output directories ($A_OUT) and compare your results to the $AGTS_L files in $ANSWERS/area/step_5/ and $ANSWERS/area/step_6/ directories, respectively.

> ***Tip***: You can use PAVE command line arguments to load the input files when you start up PAVE. For example, the following command loads the $AGTS_L file from step 4 and the $AGTS_L file in the answers directory. Note that each file name must be preceded by "-f".
>
> ```
> > pave –f $A_OUT/agts*areng* –f $ANSWERS/area/step_4/agts*areng*
> ```

In addition to comparing the files that you created during this lab with the answers, use PAVE to compare the 2-d and 3-d energy sector area-source output files.

 

You can cycle through the time steps of your $AGTS_L file using the "Animate" option in the "Control" menu. To slow down the animation, select "Set Minimum Frame Time" from the "Graphics" menu in the main window. A value of 5 is a good speed.

**Exercise 2-5:**

What is the number of the first model layer that contains emissions in the 3-d energy-sector area source output file?

**Answer 2-5:**

## 2.8 Problem solving

7. In this problem-solving exercise, you will configure SMOKE to run area sources for another grid, and using some additional options. Instead of having step-by-step instructions, you will need to figure out what files and settings are necessary. If you encounter errors along the way, you will need to figure out solutions, with the help of your instructor. You can compare your results to the answers in $ANSWERS/area/step_7/.

**Exercise 2-6:**

Configure the script and run SMOKE for area sources with the following settings:

- ☐ Process area-source emissions on the "UAE12" grid.
- ☐ Create the gridded, speciated, and temporally allocated emission files in moles/hr.
- ☐ Use cmaq5.cb05p25 speciation
- ☐ Do not create the state or county totals reports.

***Tip:*** As you have already completed all of the basic SMOKE processing steps in the previous exercises (e.g., inventory import, speciation), you only need to rerun the steps that are required for completing this problem. Think about what steps need to be rerun, and which steps do not. Discuss with your classmates or your instructor if you are unsure.

This completes the SMOKE area-sources exercise. You are now ready to move on to the third exercise, which addresses biogenic sources.

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# 3 SMOKE Training — Biogenic Sources

## 3.1 Introduction

During this biogenic emissions training, you will:

- Copy the biogenic sources run scripts, examine the scripts, and change options.
- Estimate biogenic emissions for CMAQ with the MEGAN model.
- Process using a different temperature variable from the gridded meteorology data.
- Examine biogenic emissions files in PAVE.

**NOTE:** To proceed with this lab, you must have created an Assigns file for the uae36 grid, as described in the SMOKE Overview Exercise. Use the following command to source your Assigns file:

```
> source $SMKROOT/assigns/ASSIGNS.train_<initials>.cmaq5.cb05p25.uae36
```

## 3.2 The run script and script options

1. In this step, you will copy the biogenic sources run scripts and configure them to use your Assigns file, convert gridded emissions factor and leaf area index data to netCDF files, run the **MEGAN** model, and speciate the **MEGAN** output for CMAQ.

   A. Start an xterm window (if one is not already available).

   B. Go to the directory that contains the SMOKE run scripts

   ```
   > cd $SCRIPTS/run
   ```

   C. Copy the **mg2ioapi** run script to one that uses your initials. In the instructions below, fill in your initials where indicated. Remember that you can use the tab key to complete file names.

   ```
   > cp run.mg2ioapi.mideast07.csh run.mg2ioapi_train_<initials>.csh
   ```

   D. View the **mg2ioapi** run script.

   ```
   > gedit run.mg2ioapi_train_<initials>.csh &
   ```

   E. The utility **mg2ioapi** is used to convert a text file of gridded emissions factors for biogenic sources and monthly mean leaf area index values to a binary netCDF file. Examine the script. This is a fairly simple script that sets the Assigns file, grid information, and input/output file names before calling the executable file.

   F. Change the Assigns file name to use the Assigns file that you created for the UAE36 grid in the Overview lab.

G. Save the script and execute it at the command line:

```
> run.mg2ioapi_train_<initials>.csh
```

H. Confirm that the program completed successfully by looking for the following message on your terminal window after running the script:

```
--->>  Normal Completion of program MG2IOAPI
```

If this message does not appear, check the **mg2ioapi** log file in the directory $LOGS/megan for clues about what went wrong. Fix any errors reported in the log and rerun the script before proceeding to the next step.

I. The program **MEGAN** calculates biogenic emissions using gridded emissions factors, leaf area index, land-cover, and meteorology data. Copy the **MEGAN** run script to one that uses your initials. In the instructions below, fill in your initials where indicated.

```
> cp run.megan.mideast07.csh run.megan_train_<initials>.csh
```

J. View the **MEGAN** run script. The first section of the script sets the name and location of the Assigns file and input/output directories. The second section of the script sets the dates for running the model. Note that **MEGAN** is dependent on input meteorology data. The availability of hourly meteorology will determine the time periods and spatial extent of a **MEGAN** simulation. The next part of the script sets the necessary environment variables for running and configuring the model. Within this section of the script the input and output files are defined, including the meteorology variables to use for calculating emissions.

**Exercise 3-1:**
Which environment variable controls the temperature variable to use in the MCIP output?

**Answer 3-1:**

K. Save the script and execute it at the command line:

```
> run.megan_train_<initials>.csh
```

L. Confirm that the program completed successfully by looking for the following message on your terminal window after running the script:

```
--->>  Normal Completion of program MEGAN
```

If this message does not appear, check the **MEGAN** log file in the directory $LOGS/megan for clues about what went wrong. Fix any errors reported in the log and rerun the script before proceeding to the next step.

 

M. The utility **mg2mech** converts the MEGAN output variables to the chemical species required by an air quality modeling system. This utility is the analogue of the SMOKE program Spcmat. Copy the **MEGAN** run script to one that uses your initials. Examine the new script. The first section of the script sets the name and location of the Assigns file and input/output directories. The second section of the script sets the dates of the **MEGAN** output files that will be speciated with the utility. The next part of the script sets the necessary environment variables for running and configuring **mg2mech**. Within this section of the script the input and output files are defined, along with the photochemical mechanism name to be used for the output emissions.

N. Change the Assigns file name to use the Assigns file that you created for the UAE36 grid in the Overview lab. Configure the script to create emissions using the CB05SOA mechanism.

**Exercise 3-2:**
Which environment variable did you change to set the photochemical mechanism and how did you set this variable for this exercise?

**Answer 3-2:**

O. Save the script and execute it at the command line:

```
> run.mg2mech_train_<initials>.csh
```

P. Confirm that the program completed successfully by looking for the following message on your terminal window after running the script:

```
--->>  Normal Completion of program MG2MECH
```

### *3.3 Examine the MEGAN output files with PAVE*

2. In this step you will examine the **MEGAN** output file in PAVE and create a tileplot of the pollutant ISOP (isoprene).

A. Load the **MEGAN** output file that you created and the reference output file in the $ANSWERS/step_1 directory into PAVE.

```
> pave –f $A_OUT/bgts_l.* -f $ANSWERS/biog/step_1/bgts_l.*
```

B. Compare the variables between the two files and ensure that the emissions that you generated are exactly the same as the file in the $ANSWERS directory. Create a tile plot of the isoprene emissions in the file that you created and animate the plot.

**Exercise 3-3:**
What is the value of the peak hourly isoprene emission on June 1, 2007 in the 36-km modeling grid? What time does this peak occur and in which grid cell?

**Answer 3-3:**

### *3.4 Running the biogenic model with a different temperature variable*

3. In this step you will process the biogenic emissions using ambient air temperatures.

   A. Edit the **MEGAN** run script and change the temperature variable to use the ambient air temperature (TA) in the METCRO3D file. Change the name of the **MEGAN** output file (EROUT) so that you don't overwrite the output from the previous exercise. After making these changes, save the run script.

**Exercise 3-4:**
What are the three variables that you changed in the MEGAN run script for this exercise? What are the new settings of these variables?

**Answer 3-4:**

   B. Run the **MEGAN** run script to create biogenic emissions calculated with ambient air temperatures.

```
> run.megan_train_<initials>.csh
```

   C. After confirming that **MEGAN** completed successfully, run the biogenic speciation program, **mg2mech**, to create new CMAQ emissions calculated with the alternate temperature variable. Remember to change the name of the input (MGERFILE) and output files (OUTPFILE) to read the **MEGAN** emissions computed with ambient air temperatures and to create an output file that is named differently from the file created in step 1.

   D. Run the MEGAN run script to create biogenic emissions calculated with ambient air temperatures.

```
> run.megan_train_<initials>.csh
```

 

### 3.5 Compare the MEGAN results in PAVE

4. Load the MEGAN results calculated with both the 2-m temperature and the ambient temperature variables into PAVE and compare the results. Check the results that you generated against the results in the $ANSWERS/biog/step_3 directory.

**Exercise 3-5:**
In general, how does changing from the 2-m temperatures to the ambient temperatures change the monoterpene (TERP) emissions calculated by MEGAN?

**Answer 3-5:**

### 3.6 Problem solving

5. In this problem-solving exercise, you will configure **MEGAN** to create biogenic emissions for another grid. Instead of having step-by-step instructions, you will need to figure out what files and settings are necessary. If you encounter errors along the way, you will need to figure out solutions, with the help of your instructor. You can compare your results to the answers in $ANSWERS/biog/step_5/.

**Exercise 3-6:**
Configure the MEGAN scripts to calculate biogenic emission on the "UAE12" grid.

- ☐ Convert the UAE12 emissions factor and leaf area index CSV file to netCDF.
- ☐ Compute biogenic emissions for the UAE12 grid with MEGAN. Use 2-m temperatures and solar radiation reaching the surface to calculate these emissions.
- ☐ Speciate the MEGAN emissions using the CB05SOA photochemical mechanism.

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# 4 SMOKE Training — Point Sources

## 4.1 Introduction

During this point-sources training, you will:

- Copy the point-sources run script, examine the script, and change options.
- Process point-source emissions for CMAQ.
- Project a point-source inventory to a future year.
- Examine point-source program logs and reports.
- Examine point-source emissions files in PAVE.
- Problem-solve to select elevated sources.

**NOTE:** To proceed with this lab, you must have created an Assigns file for the uae36 grid, as described in the SMOKE Overview Exercise. Use the following command to source your Assigns file:

```
> source $SMKROOT/assigns/ASSIGNS.train_<initials>.cmaq5.cb05p25.uae36
```

## 4.2 The run script and script options

1. In this step, you will copy the point-sources run script and configure it to use your Assigns file and run various point-source programs.

   A. Start an xterm window (if one is not already available).

   B. Go to the directory that contains the SMOKE run scripts:

   ```
   > cd $SCRIPTS/run
   ```

   C. Copy the point-sources script to one that uses your initials. Remember that you can use the tab key to complete file names.

   ```
   > cp smk_pt_mideast07.csh smk_pt_train_<initials>.csh
   ```

   D. View your point-sources script:

   ```
   > gedit smk_pt_train_<initials>.csh &
   ```

   E. Examine the script. At the top of the script, the SMK_SOURCE environment variable is set to “P” , indicating that point sources will be processed. Below that, the RUN_* variables control which programs will be run. Next, the program-specific and multiple-program environment variables are listed. These variables control the behavior of single programs and of two or more programs, respectively. Finally, the Assigns file is sourced and the programs are run.

F. Change the Assigns file name in the script to the Assigns file that you created for the UAE12 grid in the Overview lab.

G. Change the appropriate RUN_* environment variables to:

- ☐ Run Smkinven
- ☐ Run Grdmat
- ☐ Run Spcmcat
- ☐ Run Temporal
- ☐ Run the layer fractions program (Laypoint)
- ☐ Run Smkmerge
- ☐ Do not run emissions reporting program (Smkreport)

**Exercise 4-1:**
What were the names of the environment variables that were set to "Y" in this step?

**Answer 4-1:**

1. 2. 3.

4. 5. 6.

**Exercise 4-2:**
What environment variable is used to control the output time zone of the emissions? What is the variable set to?

**Answer 4-2:**

Variable: Value:

**Exercise 4-3:**
What environment variable is used to define the ground-level temperature variable name for plume rise computation, and what is its value?

**Answer 4-3:**

Variable: Value:

 

H. Configure the merge program to:

- ☐ Produce vertically layered output
- ☐ Create temporally allocated and speciated emissions
- ☐ Output gridded emissions in moles/s
- ☐ Output state totals from Smkmerge in moles/hr

I. Save the run script.

### 4.3 Running the point-sources script

2. In this step you will create model-ready, 3-d point source emission files.

A. Invoke the point-sources run script:

```
> smk_pt_train_<initials>.csh
```

B. While the script is running, various messages from each of the programs will scroll by on the screen. This same information is written to the log file for each program.

C. If you need to rerun a program, the script will rename your old log files rather than deleting them. This behavior is controlled by the AUTO_DELETE_LOG setting in the point-sources run script.

### 4.4 Examine the log files and output files

3. After the programs have finished, you will need to examine the log files for notes, warnings, and errors. We will also look at the report file created by Smkmerge and examine the output emissions in PAVE.

A. Go to the directory containing the log files:

```
> cd $LOGS
```

B. Confirm that all of the point-source programs completed successfully. The logs for the point-source programs will include the abbreviation "pt" in their names.

C. View the log file for the **Grdmat** program.

```
> gedit grdmat.pt.train_<initials>.UAE12.log &
```

**Exercise 4-4:**
What are the three notes that appear in this log file? (*Hint:* Search for the word "NOTE" either in gedit or using the Linux command **grep**)

**Answer 4-4:**

1.

2.

3.

Close the log file.

D. Go to the reports directory $REPSCEN to examine the report created by Smkmerge. Make sure that it is only a state totals report, and compare it to the results in $ANSWERS/point/step_3/ using either gedit or the Linux command **diff**.

E. Open a new xterm window and start PAVE. Load the gridded, speciated, hourly emissions file $PGTS3D_L (**pgts3d_l.20070601.1.UAE12.train_<initials>.ncf**) from the $P_OUT directory. You may want to use a log scale to display the emissions data; you can do this with a formula such as LOG(CO+0.0001). You can also compare your results with the file in $ANSWERS/point/step_3/.

### *4.5 Projecting point-source emissions to a future year*

4. In this section you will configure the point-sources script to grow the point-source inventory to a future year and create model-ready emissions.

   A. Go to the $SCRIPTS/run directory.

   B. Copy the future-year point-sources script to one that uses your initials:

   ```
   > cp smk_pt_mideast07_18.csh smk_pt_train_<initials>_18.csh
   ```

   C. Edit your future-year point sources script:

   ```
   > gedit smk_pt_train_<initials>_18.csh
   ```

   D. Change the Assigns file name to use the uae12 Assigns file that you created in the Overview lab.

   E. Edit the script to:

   - ☐ Run the growth matrix creation program (Cntlmat)
   - ☐ Run the program to apply the growth matrix to the inventory (Grwinven)
   - ☐ Run Temporal
   - ☐ Run Smkmerge
   - ☐ Use the same Smkmerge settings as used in Step 2; remember to set Smkmerge to output 3-D, gridded, speciated, hourly emissions and state totals

 

Save the script and exit.

F. Invoke the point-sources script:

```
> smk_pt_train_<initials>_18.csh
```

G. While the programs are running, you can look at the projection packet used by the Cntlmat program. This file is called $PTDAT/gcntl.2007_2018.txt. Each line in the file lists a FIPS code, SCC, and growth factor. The point sources will be matched to the most specific entry in the /PROJECTION/ packet.

H. After the programs have finished, confirm that they all completed successfully. The log files for Cntlmat and Grwinven are in the $LOGS directory, and the log files for Temporal and Smkmerge are in $SMKDAT/run_train_<initials>_18/static/logs.

I. Start PAVE in a new xterm window if it is not already running. Compare the base-year $PGTS3D_L file with the new $PGTS3D_L file. The 2007 $PGTS3D_L file is in the $P_OUT directory, while the 2018 $PGTS3D_L file is in $SMKDAT/run_train_<initials>_18/output/cmaq5.cb05p25 directory

You can also compare your files to those in $ANSWERS/point/step_4/.

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# 5 SMOKE Training — Processing gridded Inventories

## 5.1 Introduction

During the gridded inventories training, you will:

- Copy the biomass burning-sources run script, examine the script, and change options.
- Import a gridded biomass burning inventory into SMOKE and process it for CMAQ
- Run the layer allocation program to distribute the emissions vertically.
- Examine the gridded-inventory program logs.
- Examine biomass burning emissions files in PAVE.

**NOTE:** To proceed with this lab, you must have created an Assigns file for the uae36 grid, as described in the SMOKE Overview Exercise. Use the following command to source your Assigns file:

```
> source $SMKROOT/assigns/ASSIGNS.train_<initials>.cmaq5.cb05p25.uae36
```

## 5.2 The run script and script options

1. Copy the biomass burning-sources (bb) run script and configure it to use your Assigns file and to run inventory import, gridding, and merge.

   A. Start an xterm window if needed.

   B. Go to the directory containing the SMOKE run scripts:

   ```
   > cd $SCRIPTS/run
   ```

   C. Copy the biomass burning-sources script to one that uses your initials. Remember that you can use the tab key to complete file names.

   ```
   > cp smk_bb_mideast07.csh smk_bb_train_<initials>.csh
   ```

   D. Edit your biomass burning-sources script:

   ```
   > gedit smk_bb_train_<initials>.csh &
   ```

   E. Examine the run script. At the top of the script, the SMK_SOURCE environment variable is set to "A", indicating that the gridded inventory will be processed as an area source. Below that, the RUN_* variables control which programs will be run. Next, the program-specific and multiple-program environment variables are listed. These variables control the behavior of single programs and of two or more programs, respectively. Finally, the Assigns file is sourced and the programs are run.

F. The important setting in this script for processing gridded inventory data is the environmental variable "IMPORT_GRDIOAPI_YN". If this variable is set to "Y", then SMOKE expects that the input inventory file will be a netCDF file of gridded emissions rather than a text file of country/state/municipality total inventories.

G. Change the Assigns file name to use the uae36 Assigns file that you created in the Overview lab.

H. Configure the script to run the following steps by changing the RUN_* variables:

- ☐ Run Smkinven
- ☐ Run Grdmat
- ☐ Run Spcmat
- ☐ Run Temporal
- ☐ Run Smkmerge
- ☐ Do not run the 2-d layer allocation program (Layalloc)

I. Configure Smkmerge:

- ☐ Output a gridded file
- ☐ Produce a speciated output file
- ☐ Use moles/s for all output
- ☐ Produce temporally allocated output
- ☐ Output neither state nor country totals

Save the run script.

### 5.3 Processing gridded inventory data

2. In this step you will import the biomass burning-sources inventory, create the gridding matrix, speciation matrix, temporal intermediate files, and merge the results to create 2-d CMAQ ready emissions.

   A. Invoke the biomass burning-sources run script:

   ```
   > smk_bb_train_<initials>.csh
   ```

   B. While the script is running, various messages will be written to the screen. This same information is written to the log file for each program.

### 5.4 Examine the log files and output files

3. We will check the log files for notes, warnings, and errors, and also look at the Smkmerge report.

   A. Go to the directory with the log files:

 

```
> cd $LOGS
```

B. Confirm that all of the biomass burning-source programs completed normally by using the **tail** command on the log files.

C. View the log file for Smkinven:

```
> gedit smkinven.bb.train_<initials>.log &
```

**Exercise 5-1:**
What is the name of the inventory file used by Smkinven? Hint: we imported a gridded netCDF file, or a gridded area-source file. In SMOKE terms this is abbreviated as an "AG" file.

**Answer 5-1:**

Exit from the Smkinven log file.

D. Use PAVE to view the biomass burning gridded inventory netCDF file.

```
> pave –f  $INVDIR/gridded/ag.bb.gfedv2.UAE36LCC_148X134.2007153.8.ncf
```

Create a tileplot of the CO inventory data. Use the Control →Configure →Tile… function to bring up the plot configuration window. Change the maximum value on the legend from 4789.082 to 100.0 to see the locations of the biomass burning sources in the inventory file. After experimenting with PAVE and looking at this inventory for a few minutes, exit PAVE and move on to the next step.

E. View the log file and input files for Spcmat

```
> gedit spcmat.bb.train_<initials>.cmaq5.cb05p25.log &
```

**Exercise 5-2:**
What are the names the speciation cross reference (GSREF) and speciation profiles (GSPRO) used for the biomass burning inventory?

**Answer 5-2:**

F. Navigate to the SMOKE general data directory ($GE_DAT) and view the GSREF file used for the biomass burning inventory.

```
> cd $GE_DAT
```

```
> gedit gsref_bioburn.txt &
```

This GSREF file contains one entry for each pollutant in the biomass burning inventory and uses the default SCC code "0000000000" to identify the source for each profile. Because gridded inventories do not contain source-specific identification information, such as FIPS codes and SCC's, the normal hierarchical cross-referencing that SMOKE uses for applying profiles does not work. As such, only a single speciation profile can be applied to each pollutant in a gridded inventory. Similarly, a single temporal profile will be applied uniformly across all of the grid cells in a gridded inventory.

The speciation and temporal cross-reference and profile files used with gridded inventories MUST CONTAIN ONLY A SINGLE ENTRY. Only one set of profiles per cross-reference and profile file is allowed for processing gridded inventories. The SCC field of the cross-reference files must contain the fallback or default code of all zeros (0000000000).

To process multiple gridded inventories (i.e. biomass burning, commercial shipping, industrial area, on-road mobile, etc.), you must run each inventory through SMOKE separately. Source-specific speciation and temporal cross-reference and profile files will also need to be developed and applied to each explicit gridded inventory.

Close the GSREF file.

G. Navigate to the output data directory and view the processed biomass burning inventory in PAVE.

```
> pave –f $A_OUT/bbgts_l*
```

Use PAVE to explore the biomass burning processed emissions data. Note that all of the emissions are allocated to layer 1 only. In the next exercise we will distribute these emissions to the vertical model layers.

### *5.5 Generate 3-d emissions data*

4. In this step, you will run the SMOKE utility **Layalloc** to distribute the biomass burning emissions to the vertical model layers.

   A. Go to the directory containing the SMOKE run scripts:

   ```
   > cd $SCRIPTS/run
   ```

   B. Configure the biomass burning script to run the following steps by changing the RUN_* variables:
   - ☐ Do not run Smkinven
   - ☐ Do not run Grdmat
   - ☐ Do not run Spcmat
   - ☐ Do not run Temporal

 

- ☐ Do not run Smkmerge
- ☐ Run Layalloc

Save the biomass burning run script.

C. Navigate to the GE_DAT directory and open the biomass burning LAYER_FRACTION file.

```
> cd $GE_DAT

> gedit layers_gfed.txt &
```

**Exercise 5-3:**
What percentage of the biomass burning emissions will be allocated to the altitude band from 0 – 50m? What is the maximum emission height specified for biomass burning by this LAYER_FRACTION file?

**Answer 5-3:**

Exit from the LAYER_FRACTION file after completing the exercise.

D. Navigate back to the $SCRIPTS/run directory and execute the biomass burning run script.

```
> smk_bb_train_<initials>.csh
```

### *5.6 Compare the 2-d and 3-d emissions*

5. In this step, you will load the 2-d and 3-d biomass burning emissions files into PAVE and compare the results.

A. Load the biomass burning data into PAVE.

```
> pave –f $A_OUT/bbgts_l.* -f $A_OUT/bbgts3d_l.*
```

**Exercise 5-4:**
What is the highest model layer into which the biomass burning emissions are allocated? What's the maximum hourly NO emissions estimate in this layer?

**Answer 5-4:**

## 5.7 Problem solving

6. In this problem-solving exercise you will rerun the layer allocation step for the biomass burning sources after changing the vertical profiles for these sources. Create a new biomass burning emission file with the following vertical distribution:

| Altitude Band (m) | % Emissions |
|---|---|
| 0-25 | 10 |
| 25-75 | 15 |
| 75-500 | 60 |
| 500-1500 | 15 |

Instead of following step-by-step detailed instructions, you will need to figure out what files and settings are needed to accomplish this task. If you encounter errors along the way, you will need to figure out solutions, with the help of your instructor. You can compare your results to the answers in $ANSWERS/gridded/step_6/.

**Exercise 5-5:**

Use the SMOKE utility Layalloc to create new 36-km biomass burning emissions using an alternative vertical allocation profile. Things to consider when setting up this case include:

- Creating a new LAYER_FRACTION file in the GE_DAT directory
- Changing the LAYER_FRACTION file for biomass burning (bb) in the 36-km Assigns file
- Renaming the previous biomass burning 3-d emissions file (use the Unix command ‘mv’ to rename the file).

 

# 6 SMOKE Training — Merging

## 6.1 Introduction

During this merge processing training, you will:

- Copy the merge run script, examine the script, and change options.
- Use the SMOKE merge tool (Mrggrid) to combine model-ready files.

**NOTE:** To proceed with this lab, you must have created an Assigns file for the uae36 grid, as described in the SMOKE Overview Exercise. Use the following command to source your Assigns file:

```
> source $SMKROOT/assigns/ASSIGNS.train_<initials>.cmaq5.cb05p25.uae36
```

## 6.2 The run script and script options

1. Copy the merge (mrgall) run script and configure it to use your Assigns file.

   A. Start an xterm window if needed.

   B. Go to the $SCRIPTS/run directory.

   C. Copy the merge script to one that uses your initials:

   ```
   > cp smk_mrgall_mideast07.csh smk_mrgall_train_<initials>.csh
   ```

   D. Edit your merge script in gedit and change the Assigns file setting to use your 36-km Assigns file:

   ```
   > gedit smk_mrgall_train_<initials>.csh
   ```

## 6.3 Using the Mrggrid program

2. The **Mrggrid** program lets you merge together previously created model-ready files without needing the intermediate files from the various SMOKE programs. We will use the **Mrggrid** program to combine 2-d area-, 3-d area-, 3-d gridded-, and biogenic emissions that you created previously into a single output file.

   A. Set the script to run the gridded file merge program (Mrggrid)

   B. Look at the section of the script labeled “Script Settings”. There are three environment variables that we need to set in this section: MRGFILES, MRGGRID_MOLE, and SRCABBR.

- ☐ Set the MRGFILES environment variable to "ARGTS_L BBGTS3D_L AENGGTS3D_L BGGTS_L" to merge the area-, biomass burning-, area energy- and biogenic-source model-ready files that we created.
- ☐ Set MRGGRID_MOLE to "Y" to match the units of the MRGFILES files (moles).
- ☐ Set SRCABBR to match the source types we are merging (area+biogenic+biomass burning = arbgbb).

C. Save the merge script.

D. From the $SCRIPTS/run directory, execute the merge script:

```
> smk_mrgall_train_<initials>.csh
```

### 6.4 Confirm that Mrggrid worked

3. Start PAVE if it is not already running. Load the $ARGTS_L, $AENGTS3D_L, $BBGTS3D_L, $BGGTS_L and $EGTS_L files from their respective output directories. Create a formula for NO that subtracts the component emissions from the combined file, and plot this formula. The results should be close to zero everywhere.

   You can check other species in the various files and compare them to the $EGTS_L file created in Step 2. You can also compare your log files and results with those in $ANSWERS/merge/step_2/.

### 6.5 Create a biomass-burning emissions sensitivity case

4. In this exercise you will rerun the program **Mrggrid** program to combine all of the files from the previous step, except for biomass burning emissions. Removing one emissions sector from an emission simulation is one way to determine the sensitivity of air quality to the emissions from that sector. Comparing the result of a pair of air quality model simulations, one with and the other without biomass burning emissions, will demonstrate the impacts of biomass burning on air quality. This exercise demonstrates how to set-up a "brute-force" emissions sensitivity for air quality modeling.

   A. Edit the merge script that you created in Step 2 to create merged emissions that do not include biomass burning data. Set the MRGFILES environment variable to "ARGTS_L AENGGTS_L BGGTS_L". Notice how you removed the variable BBGTS3D_L from the list created previously. Also change the SRCABBR environment variable to reflect that the emissions only contain area and biogenic sources (arbg).

      Save the script and exit from the text editor.

   B. Go the $OUTPUT directory and rename the previous SMOKE output file.

      ```
      > cd $OUTPUT
      ```

 

```
> mv egts_l.20070601.1.UAE36.train_<initials>.ncf
egts_l.20070601.1.UAE36.train_<initials>.ncf_bb
```

C. Return to the $SCRIPTS/run directory and execute the merge script.

```
> cd $SCRIPTS/run
> smk_mrgall_train_<initials>.csh
```

### 6.6 Compare the SMOKE output files in PAVE

5. Start PAVE if it is not already running. Load the $EGTS_L files with and without biomass burning emissions from the output directories. Create a formula for NO that subtracts the emissions without biomass burning sources from the emissions file that includes these sources. You can also load in the biomass burning data file from the $A_OUT directory into PAVE and compare the NO emissions in this file with the NO difference between the merged files. The merged file difference and the biomass burning-only data should be exactly the same.

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# 7 SMOKE Training — Quality Assurance

## 7.1 Introduction

During this quality assurance training, you will:

- Turn on the quality assurance options in some of the scripts you have already run.
- Review quality assurance reports to check processing.
- Build a new quality assurance configuration file with explicit instructions.
- Build a new quality assurance configuration file as a problem-solving exercise.

**NOTE:** To proceed with this lab, you must have created an Assigns file for the uae36 grid, as described in the SMOKE Overview Exercise. Use the following command to source your Assigns file:

```
> source $SMKROOT/assigns/ASSIGNS.train_<initials>.cmaq5.cb05p25.uae36
```

## 7.2 The quality assurance script options

1. Turn on the area-source quality assurance script options.

   A. Go to the $SCRIPTS/run directory.

   B. View your area-sources script:

   ```
   > gedit smk_ar_train_<initials>.csh &
   ```

   C. Configure the script to:

   - ☐ Use the 36-km Assigns file
   - ☐ Do not rerun any area-source processing steps
   - ☐ Run the emissions reporting program (Smkreport)
   - ☐ Create inventory reports by setting QA_TYPE to "part1"

   The following settings are valid for the QA_TYPE setting: "none", "all", "part1", "part2", "part3", "part4", and "custom". Note that "part3" and "part4" are used only for point-source quality assurance. The qa_run.csh script sets which reports will be created for each QA_TYPE setting.

   D. Save the run script.

### 7.3 Run the reporting program for area sources

2. Now you will run the script that you created in the previous step, and then look at the reports generated from this run.

   A. Invoke the area-sources script.

   ```
   > smk_ar_train_<initials>.csh
   ```

   B. All the reports created by QA_TYPE "part1" will go in the $REPSTAT directory. Go to this directory and open the inventory reports.

   ```
   > cd $REPSTAT
   > gedit a*.rpt &
   ```

**Exercise 7-1:**
Which SCC in the area-source inventory has the largest total CO emissions, and what is the name of that SCC?

**Answer 7-1:**

SCC:

Name:

### 7.4 Run the reporting program for point sources

3. In this step you will run the quality assurance option for the point-sources script that you have already worked with.

   A. Go to the directory that contains the SMOKE run scripts:

   ```
   > cd $SCRIPTS/run
   ```

   B. View your point-sources script:

   ```
   > gedit smk_pt_train_<initials>.csh &
   ```

   C. Configure the script to:

   - ☐ Use the 12-km Assigns file
   - ☐ Do not rerun any point-source processing steps
   - ☐ Run the emissions reporting program
   - ☐ Create all point-source reports by setting QA_TYPE to "all"

   D. Invoke the point-sources script.

 

E. Reports using temporalized emissions will go in the $REPSCEN directory, while time-independent reports will be put in the $REPSTAT directory.

F. Once the reports have been generated, go to the $LOGS directory.

**Exercise 7-2:**
How many times did Smkreport run? How many times did it complete successfully? If it failed what was the ERROR message reported by SMOKE?

**Answer 7-2:**

G. Examine and compare the reports in the $REPSTAT and $REPSCEN directories.

**Exercise 7-3:**
Look in the report by SCC and by hour in the $REPSCEN directory. How many tons/hr of NOx are emitted by SCC 20100201 on hour 17?

**Answer 7-3:**

### *7.5 Run the quality assurance step for area sources using a custom configuration*

4. In this step you will follow a specific set of instructions to create a REPCONFIG input file that you will use to create a custom area-sources report. To create the REPCONFIG file, you may need to review the format of this file in Section 7.3 of the SMOKE User's Manual. You can also look at existing REPCONFIG files in the $INVDIR/other directory.

   A. Return to the $SCRIPTS/run directory and open the mobile-sources script that you created previously:

```
> cd $SCRIPTS/run
> gedit smk_ar_train_<initials>.csh
```

   B. Configure the script to:

   - ☐ Use the 36-km Assigns file
   - ☐ Do not rerun any area-source processing steps
   - ☐ Run the reporting program

- ☐ Set QA_TYPE to "custom"
- ☐ Make a new environment variable REPORT1 under the "Script settings" section of the script and set it to $REPSCEN/ar.custom.rpt

C. Save the area-sources script.

D. Create a new file in the $ARDAT directory called repconfig.area.txt.

E. In this REPCONFIG file, enter the commands to:

- ☐ Run for area sources
- ☐ Create REPORT1
- ☐ Include gridding
- ☐ Include temporal allocation
- ☐ Report by state name
- ☐ Report by grid cell
- ☐ Report by hour
- ☐ Report in units of g/hr
- ☐ Report emissions using float format with 1 decimal place and columns that are 12 spaces wide

F. Save the report configuration file.

G. From the $SCRIPTS/run directory, run the area-sources script.

```
> smk_ar_train_<initials>.csh
```

H. Confirm that Smkreport completed normally by looking at the log file in $LOGS. Then, verify that your custom report was created in the $REPSCEN directory, and that it matches the description given above.

 

# SMOKE Version 3.1i Training Answer Sheet

| | |
|---|---|
| 1-1 | ABASE |
| 1-2 | $GE_DAT/gspro.cmaq5.cb05p25.txt |
| 1-3 | ESCEN |
| 1-4 | • EPI_STDATE: 2007152<br>• EPI_STTIME: 000000<br>• EPI_RUNLEN: 0240000<br>• EPI_NDAY: 1<br>• G_STDATE: 2007152<br>• G_STTIME: 000000<br>• G_RUNLEN: 250000<br>• ESDATE: 20070601<br>• NDAYS: 1 |
| 2-1 | 1. RUN_SMKINVEN 2. RUN_GRDMAT 3. RUN_SMKMERGE |
| 2-2 | 1. MRG_GRDOUT_YN 2. MRG_REPCNY_YN<br>3. MRG_REPSTA_YN 4. MRG_GRDOUT_UNIT<br>5. MRG_TOTOUT_UNIT 6. MRG_TEMPORAL_YN<br>7. MRG_SPCMAT_YN |
| 2-3 | 1. Missing [inventory field] for [pollutant] at line ##<br>2. Missing SIC code at line [line number]. Default 0000 will be used.<br>3. No kept pollutant found at line [line number].The source will be dropped.<br>4. Some base year control efficiency values that were input as 100%<br>5. Some base year rule effectiveness values that were input as 0% |
| 2-4 | 546; the number of sources in the inventory |
| 2-5 | Layer 5 |
| 2-6 | Solution for problem (Area Source with new 12 km grid)<br>1. Change 36km Assign file to the 12km Assigns file name that you created in the Overview Lab.<br>2. RUN_GRDMAT = Y<br>Since it is for 12km, you need to re-run GRDMAT but there is no need to run Smkinven, Spcmat, or Temporal<br>3. Run_SMKMERGE = Y<br>• MRG_SPCMAT_YN Y<br>• MRG_TEMPORAL_YN Y<br>• MRG_GRDOUT_YN Y<br>• MRG_REPCNY_YN N<br>• MRG_REPSTA_YN N<br>• MRG_GRDOUT_UNIT moles/hr<br>• MRG_TOTOUT_UNIT moles/yr |
| 3-1 | TEMPVAR |
| 3-2 | MECHANISM, CB05SOA |
| 3-3 | 78.691 moles/s at hour 12:00 in cell (3,24) |

| | |
|---|---|
| 3-4 | EROUT = $INTDIR/ER_MEGAN_UAE36k_148X134_${SDATE}_TA.ncf<br>TMPFILE = $METDIR/METCRO3D_$SDATE<br>TEMPVAR = TA |
| 3-5 | The 2-m temperatures produce higher emissions estimates during day while the ambient temperatures produce higher emissions estimates at night. |
| 3-6 | Solution for problem (Biogenic sources on the 12 km grid)<br>• Change the name of the Assigns file in the mg2ioapi script to the 12-km file.<br>• Check the name of the 12-km grid in the $GE_DAT/GRIDDESC file<br>• Set the GDNAM3D variable in the mg2ioapi script to UAE12LCC_78X72.<br>• Change the names of the input (INPFILE) and output (OUTFILE) files in the mg2ioapi script to refer to the 12-km grid name.<br>• Change the log file name in the mg2ioapi script to create file tagged with "uae12" instead of "uae36".<br>• Change the name of the Assigns file in the MEGAN script to the 12-km file.<br>• Change the names of the input (ECMAP) and output (EROUT) files in the MEGAN script to refer to the 12-km grid.<br>• Change the temperature file (TMPFILE) to use the METCRO2D file in the MEGAN script.<br>• Change the air temperature variable to 2-m temperatures (TEMP2) in the MEGAN script.<br>• Change the log file name in the MEGAN script to create file tagged with "uae12" instead of "uae36".<br>• Change the name of the Assigns file in the mg2mech script to the 12-km file.<br>• Change the names of the input (MGERFILE)/(PFTFFILE) and output (OUTPFILE) files in the mg2mech script to refer to the 12-km grid.<br>• Change the log file name in the mg2mech script to create file tagged with "uae12" instead of "uae36". |
| 4-1 | 1. RUN_SMKINVEN 2. RUN_GRDMAT 3. RUN_SPCMAT<br>4. RUN_TEMPORAL 5. RUN_LAYPOINT 6. RUN_SMKMERGE |
| 4-2 | Variable: OUTZONE Value: 0 |
| 4-3 | Variable: PLUME_GTEMP_NAME Value: TEMP2 |
| 4-4 | 1. Grid settings initialized using UAE12LCC_78X72 in grid description file<br>2. Output grid "UAE12LCC_78X72" set; described as<br>3. Number of sources excluded from grid was 0 |
| 5-1 | ag.bb.gfedv2.UAE36LCC_148X134.2007153.8.ncf |
| 5-2 | GSREF = gsref_bioburn.txt, GSPRO = gspro_bioburn.txt |
| 5-3 | 25%, 2000 m |
| 5-4 | Layer 19, 0.031 moles/s |
| 5-5 | Solution for the problem to create a new vertical distribution profile for biomass burning emissions.<br>• Create a new LAYER_FRACTION file with the layer distribution information provided for this exercise<br>• Change the LAYER_FRACTION environment variable on line 108 of the 36-km Assigns file to point to the new file. |

 

| | |
|---|---|
| | • Rename the biomass burning 3-d output file in the $A_OUT directory to a new file name so that this file does not get overwritten during this exercise.<br>• Run the biomass burning script with only the RUN_LAYALLOC variable set to "Y". All other RUN variables should be set to "N". |
| 7-1 | SCC: 99CIRCERES<br>Name: CIRCE Residential |
| 7-2 | Smkreport ran 3 times and it completed 2 runs; there was an error in the elevpoint report that SMOKE could not open the input file "PELV" |
| 7-3 | 11.077 tons/hour |