Chapter 8. SMOKE Quality Assurance and Utility Programs

Contents

Overview

Beld3to2 program converts BELD3 netCDF files into an ASCII BELD2 file for input into Rawbio

Metscan will read up to one year of first-layer I/O API meteorology (whether 2-d or 3-d files) and determine the first and last freeze dates of the year for use by Tmpbio in setting winter/summer emission factors by day and grid cell.

Mvcondns will read a Smkinven output MOBL file and created a condensed list of all sources in the inventory by country/state/county code, roadtype, vehicle type, and including the speed from the inventory if any is available. Determines a default speed for each county and road type.

Mvsetup will create the MPLIST file using the output from Mvcondns and other supplementary information.

Pktreduc will reduce the size of projection packets, but keeps the same information by identifying and implementing state defaults where none already exist in the file.

Smkreport is a general reporting program for SMOKE. It has a lot of different configuration options to generate many types of reports for quality assurance purposes.

The **Smk2emis** program converts SMOKE netCDF files into a UAM or CAMx-ready emissions file.

Surgtool can input SMOKE-formatted gridding surrogates for a "fine" input and output a surrogate file for a "coarse" output file. It produces approximate "coarse" grid surrogates, the accuracy of which depends on how fine the reolution of the input grid is relative to that of the output grid.

The **Uam2ncf** converts UAM ready emissions files into netCDF format.

BELD3TO2

Description

Beld3to2 reads in the Biogenic Emissions Landcover Database version 3 (BELD3) data in netCDF (typically created by the MODELS-3 SMOKE Tool). The BELD3 consists of 230 land use types. Since IOAPI has a limit of 120 variables that can go in one netCDF file, the BELD3 landuse data read in must be contained in two land use files. An additional input file that contains the amount of land use data obtained from the Forest Inventory Area (FIA) database is used. This FIA data is mainly important when converting land use data over Canada. Since Rawbio only understands BELD version 2 (BELD2) land use types (127 different land use types), BELD3TO2 also reads in a cross-reference file, B3XRF, that converts the 230 BELD3 land use types into the 127 BELD2 land use types. The output from this program is a gridded ASCII land use file ready for input into Rawbio. The grid characteristics of the output file are obtained from the BELD3 land use files. The grid characteristics are then output at the top of the BGUSE file on the #GRID line (usually the first line).

Processing Order

If the user does not have gridded landuse for use in SMOKE-BEIS2 (Rawbio and Tmpbio), the user can use the MODELS-3 SMOKE tool to generate BELD3 data in netCDF. Then execute Beld3to2 with this BELD3 data as input. The output from this program, BGUSE, can be used in Rawbio.

Input Files

File Name	Description
BELD3_A	(I/OAPI netCDF) BELD3 landuse data file A (first 120 land use types)
BELD3_B	(I/O API netCDF) BELD3 landuse data file B (remaining 110 land use types)
BELD3_TOT	(I/O API netCDF) BELD3 landuse totals file: contains additional information about the BELD3 data for the same modeling domain in the BELD3_A and BELD3_B files
B3XRF	(ASCII) Cross-reference file that maps the BELD3 land use types to the BELD2 land use types

Input Environment Variables

- **None**

Output Files

- **BGUSE:** (ASCII) gridded land use data in ASCII format containing BELD2 land use types.
- **LOGFILE:** (ASCII) This file contains the log generated from executing this program.

Earlier Versions

Please note that the B3XRF file has been updated with the SMOKEv1.4 beta release. The earlier version of this file had only been tested in the eastern United States. Application of this program for the rest of North America (BELD3 geographical area) resulted in numerous changes to the B3XRF file.

METSCAN

Description

Metscan reads in the an annual temperature I/O API meteorology file and determines the first freeze date and last freeze date of a year, by grid cell. It outputs a gridded file with a daily time step that has a value of zero for winter cells and a value of 1 for summer cells. The program can be set to run in the northern hemisphere or in the southern hemisphere and will not work on global meteorology datasets. In the northern hemisphere, the first freeze date in the fall marks the start of winter, and the last freeze date in the spring marks the end of winter. All other days are considered summer days, since the BEIS2 and BEIS3 models operate using the assumption of either winter or summer emission factors.

Processing Order

Metscan can optionally be used before Tmpbio, which does not require the output from Metscan to run. Metscan is only needed when users wish to have Tmpbio automatically switch between winter and summer emission factors by grid cell.

Input Files

File Name	Description
MET_CRO_3D	Annual meteorology file. This can be a 2-d or 3-d file (though the logical file name is the same). The file can be created by extracting temperature variables out of the MET_CRO_2D or MET_CRO_3D files output by the MCIP or MCPL programs using the m3xtract I/O API utility and appending all days of data into the same file.

Input Environment Variables

- **TMPR_VAR:** Default [TA]. Sets the name of the temperature variable that will be read from the MET_CRO_3D input file. Acceptable values for MCIP and MPCL outputs available at the time of this writing are TA (ambient layer-1 temperature from the MET_CRO_3D file), TEMP10 (10-meter temperature from the MET_CRO_2D file), TGD (ground temperature), TGRND (ground temperature), and TEMP15 (1.5 meter temperature).

- **N_S_HEMI:** Default [NORTH]. Sets the program to run for the Northern or Southern hemisphere. Acceptable values for this setting are:

- NORTH: Northern hemisphere
- SOUTH: Southern hemisphere

Output Files

- **BIOSEASON**: (I/O API NetCDF) This file contains the 0 for winter grid cells and days, 1 for summer (non-winter) grid cells and days. Its duration will be as long as the input meteorology file provided.
- **LOGFILE:** (ASCII) This file contains the log generated from executing this program.

MVCONDNS

Documentation on this program will be included with the final SMOKE version 1.4 release.

MVSETUP

Documentation on this program will be included with the final SMOKE version 1.4 release.

PKTREDUC

Documentation on this program will be included with the final SMOKE version 1.4 release.

SMK2EMIS

Description

Smk2emis converts SMOKE NetCDF gridded, speciated, hourly emissions into the Fortran-binary format used for 2-d emissions by UAM-IV, UAM-V, CAM_X, and REMSAD. Files of this format use the UAM keyword "EMISSIONS". The SMOKE user is responsible for preparing the NetCDF inputs with the appropriate chemical species, grid structures, time steps, and units for use in whatever model will be used with the results of Smk2emis.

Processing Order

The Smk2emis program will input the netCDF gridded, mole-speciated, hourly emissions files output from Smkmerge (AGTS_L, MGTS_L, PGTS_L, or EGTS_L) or output from Tmpbio (BGTS_L). Therefore, Smk2emis must be run after Smkmerge and/or Tmpbio.

Input Files

File Name	Source Type	Description
[A|B|M|P|E]GTS_L	A, B, M, P, All	I/O API SMOKE gridded, speciated, hourly emissions file
VNAMMAP	A, B, M, P, All	Optional ASCII file for renaming variables from those in the I/O API file header to those needed by the air quality model. See the SMK2EMIS_VMAP_YN environment variable

Input Environment Variables

- **FLABEL:** [default EMISSIONS]
  Defines what type UAM/CAMx file to output
    - EMISSIONS: Gridded, hourly emissions; only working option
- **SMK2EMIS_VMAP_YN** : [default: N]
  Controls whether the name remapping file will be read in, to output different variable names from Smk2emis than are in the input file. This is needed for using UAM-AERO, which requires symbols in the variable names (such as ".", "+", and "-") that are not permitted in I/O API file variable names.

  - Y: Use the VNAMMAP file
  - N: Do not use the VNAMMAP file

- **SMK_SOURCE:** see Chapter 5, section on Shared Environment Variables. This variable controls the name of the input NetCDF logical file name and the name of the output binary logical file name. Unlike most other SMOKE programs, SMK_SOURCE can also be set to "E" for this program to indicate that the "every" source category merged file should be converted from NetCDF to UAM binary format.

- **UTM_ZONE:** [default -9]
  Defines UTM zone for the header of the UAM EMISSIONS file.
  - -9: Latitude-longitude projection

- **UAM_LAYERS:** [default NLAYS3D]
  Defines number of layers in output file
  - NLAYS3D: value from SMOKE netCDF input file

- **UAM4_LAYBELOW:** [default 0]
  Defines number of layers below diffusion break
  - 0: UAM-V or CAMx style
  - >0 : UAM-IV style

- **UAM4_LAYABOVE:** [default 0]
  Defines number of layers below diffusion break
  - 0: UAM-V or CAMx style
  - >0 : UAM-IV style

- **UAM4_HTSFC:** [default: 0.0]
  Defines height of surface layer
  - 0.0: UAM-V or CAMx style
  - >=0.0: UAM-IV style

- **UAM4_HTLOWR:** [default: 0.0]
  Defines minimum height of cells between surface layer and diffusion break (meters)

  - 0.0: UAM-V or CAMx style
  - >0.0: UAM-IV

- **UAM4_HTUPPR:** [default: 0.0]
  Defines minimum height of cells between diffusion break and top of region(meters)
  - 0.0: UAM-V or CAMx style
  - >0.0: UAM-IV

- **UAM_NOTE:** [default: UAM gridded emissions from SMK2EMIS]
  Defines the note to be written to the header of the UAM output file

Other Input

When running Smk2emisS interactively, the following inputs will be requested. The default values for these are set by the time variables found in the input NetCDF file header. If not running Smk2emis interactively, the values of these settings will be taken from the input file being converted to UAM-V format.

- **Start date:** Starting date of simulation in Julian (DDDYYYY) or Gregorian (MMDDYYYY) formats
- **Start Time:** Starting time of simulation in HHMMSS.
- **Duration:** Simulation duration in hours.

Output Files

- **UAM_[A|B|M|P|E]GTS:** (Fortran binary) UAM-IV, UAM-V or CAMx-ready gridded, hourly emissions.
- **LOGFILE:** (ASCII) This file contains the log generated from executing this program.

Earlier Versions

~~The SMOKE prototype used a USERIN file to input the necessary UAM header information.~~ The USERIN file is no longer needed.

SMKREPORT

Description

Smkreport uses the SMOKE intermediate files generated by other SMOKE programs to create a large variety of emissions and activity data totals to be used for further QA of the emissions data. Smkreport operates on **one** source category (area, mobile, or point) in a given run. Each run of Smkreport is also limited to one speciation scenario, one grid, and one hourly emissions file. Smkreport cannot yet read in projection or control matrices. All of these component datasets are optional, however, and their use is controlled by the settings in the Report Configuration File (REPCONFIG). Analysis of multiple source categories together will remain, for now, as a post-processing step in which the user can import multiple reports from different source categories and analyze across multiple source categories.

The most important input file is the Report Configuration File. Through this file, the user has a tremendous amount of flexibility in generating different types of reports. Options are invoked by using reporting "Instructions," which the user prepares before using Smkreport. Please see the REPCONFIG documentation for more information on the reporting options.

Smkreport can generate multiple reports with a single run of the program. Multiple report writing is helpful, because a large part of the time that the program takes to run is reading in the SMOKE intermediate files. Note that the multiple reports are all for a single source category for one run of the Smkreport program.

Processing Order

Smkreport can only be used after at *least* Smkinven (for inventory import) has been run. Depending on the reporting options selected in the REPCONFIG input file, other processing steps may need to have been run. For example, to create a report of county total emissions after gridding, the Grdmat (for spatial allocation) program must have been run already to create the gridding matrix. Smkreport can use output files from the following programs: Smkinven, Temporal (for temporal allocation), Spcmat (for chemical speciation), Grdmat, Elevpoint (for elevated source selection), Laypoint (for plume rise calculations), and Cntlmat.

Input Files

The input files depend upon the SMK_SOURCE input instruction in the REPCONFIG input file setting when the program is started. For example, if only area sources are being merged (SMK_SOURCE=A), then only area source-related inputs are required. Similarly, if Smkreport is being executed to produce speciated, gridded, temporally allocated area sources, then the area-source inventory, speciation matrix, gridding matrix, and hourly emissions are required.

File Name	Source Type	Description
[A|M|P]CMAT	A, M, P	multiplicative control matrix in I/O API netCDF format (optional, *not yet supported by SMOKE*)
[A|M|P]GMAT	A, M, P	gridding matrix from Grdmat in I/O API netCDF format (optional)
[A|M|P]GSUP	A, M	Supplementary file from Grdmat that contains all gridding surrogate codes assigned to each source
[A|M|P]RMAT	A, M, P	mass-based or mole-based reactivity matrix from Spcmat in I/O API netCDF format (optional, *not yet supported by SMOKE*)
[A|M|P]SMAT	A, M, P	mass-based or mole-based speciation matrix from Spcmat in I/O API netCDF format (optional)
[A|M|P]SSUP	A, M, P	Supplementary file from Spcmat that contains all speciation profile codes assigned to each source
[A|M|P]SRC	A, M, P	SMOKE emissions character-string inventory information from Smkinven in ASCII format (optional)
[A|M|P]TMP	A, M, P	temporally allocated emissions from Temporal in I/O API netCDF format (optional)
[A|M|P]TSUP	A, M, P	Supplementary file from Temporal that contains all monthly, weekly, and diurnal profile codes assigned to each source. **This file will only work when profiles have not been applied by pollutant.**
AREA	A	SMOKE area source emissions inventory with numeric data only from Smkinven program in I/O API netCDF format (optional)
COSTCY	A, M, P	country, state and county file with time zones and optionally population (optional)
G_GRIDPATH	A, M, P	contains description of the modeling grid in ASCII format

MOBL	M	SMOKE mobile source emissions inventory with numeric data only from Smkinven program in I/O API netCDF format (optional)
PELV	P	elevated point sources identification file; if reporting based on elevated point sources (optional)
PLAY	P	SMOKE layer fractions file in I/O API netCDF format, output by the Laypoint program (optional)
PNTS	P	SMOKE point source emissions inventory with numeric data only from Smkinven program in I/O API netCDF format (optional)
REPCONFIG	A, M, P	Report configuration file in ASCII format
SCCDESC	A, M, P	SCC descriptions

Input Environment Variables

- None

Output Files

- **REPORT[#]:** (ASCII) Multiple ASCII reports. Smkreport will output file names of REPORT1, REPORT2, REPORT3, etc., if no other file names are given with the /NEWFILE/ instruction (see the REPCONFIG file documentation). If the /NEWFILE/ instructions include physical file names, Smkreport will open those files. If the /NEWFILE/ instructions include logical file names, Smkreport will attempt to find the value of the logical file name in the environment. It the logical file name is defined, Smkreport will open the physical file it has been defined to; otherwise Smkreport opens a physical file with the same name as the logical file name.

- **LOGFILE:** (ASCII) This file contains the log generated from executing this program.

SURGTOOL

Documentation on this program will be included with the final SMOKE version 1.4 release.

UAM2NCF

Description

Takes UAM EMISSIONS gridded files and creates NetCDF gridded file which can be merge with other gridded SMOKE netCDF files.

Processing Order

Input Files

File Name	Source Type	Description
UAMEMIS	Optional	UAM ready, Fortran-binary, gridded emissions file.

Input Environment Variables

Other Input

Output Files

- **E2DNCF:** Gridded, hourly emissions in netCDF format.
- **LOGFILE:** (ASCII) This file contains the log generated from executing this program.
