Chapter 3. Source-category-specific concepts

Contents

Introduction

Emissions processing for air quality modeling is divided into four types of sources: area, biogenic, mobile, and point. This chapter provides a description of each of these types of sources and describes their processing requirements.

Area Source Processing

The essence of area source emissions processing in SMOKE is converting inventory pollutant data for counties and source categories from aggregated annual or average daily emissions value to hourly and gridded emissions of the chemical species used by an air quality model. The SMOKE processing can be run with or without control strategies. The system accepts raw data in IDA and EMS-95 formats, and it has been designed for future implementation of EPS2.0.

Because area sources are the least complex source category, they are a good starting point for someone who is unfamiliar with the SMOKE system.

In addition to inventory import, the remaining area source processing steps are speciation, temporal allocation, projection, control, and gridding. These are implemented using the standard emissions cross-reference and profile approach in which each county and source category code (SCC) code is indirectly assigned a profile number by using a cross-reference file. A given profile number is used to find the appropriate temporal profile, speciation profile, etc., that transform the raw data using factors from the profiles.

The following identifiers define SMOKE area sources: country/state/county code and source classification code.

SMOKE can combine raw data from different inventory years into a single inventory. The

inventory year is stored as one of the records in the SMOKE area source inventory file AREA. The data from these different years can then be projected to the same year using the Cntlmat projection and controls program. The projection inputs for the Cntlmat have been set up so that the projection factors are listed with the "from year" and the "to year".

There are many other features for area source processing, which are documented in the SMOKE Core Programs Chapter. The relevant SMOKE programs are Smkinven, Spcmat, Grdmat, Temporal, Smkmerge, Grwinven, and Mrggrid. The various options for the SMOKE programs are usually applicable to area source emissions.

Biogenic

SMOKE biogenic emissions modeling, "SMOKE-BEIS2," is an adaptation of BEIS2 to fit within the data flows of SMOKE and to work compatibly with the meteorology and air quality models being developed with EDSS and Models-3.

There are two different paths of processing for SMOKE-BEIS2, depending upon whether one begins with gridded or county-aggregated BEIS2 land use data. Both produce the same sort of gridded normalized biogenic emissions output file BGRD, which contains gridded land use type specific normalized (time-independent) emissions and biomass data.

First is the the county-aggregated landuse case. Program Rawbio reads a county list from the BFIP file, BEIS2 county-aggregated land use data from the BCUSE file, BEIS2 emissions factors from the BFAC file, and gridding-surrogate coefficients from BGPRO to produce this file. Alternatively, Rawbio can import a gridded land use data file, BGUSE. The processing is the same as for county land use, except the gridding surrogates are not needed for grid cell allocation of the emissions. In both cases, BGRD then goes into Tmpbio to prepare model-ready biogenic emissions.

It is possible for the user to define the chemical species that are output from Tmpbio. This is possible because Tmpbio has been updated to read the speciation profiles file, GSPRO. The user then sets an environment variable indicating which speciation profile should be used for biogenic emissions. Tmpbio looks for the “inventory pollutants” OVOC, NO, and TERP, and splits and/or aggregates these data as specified by the profile.

SMOKEv1.4 introduced a BEIS3 prototype, BEIS v3.09. The concepts in BEIS3 are similar to those in BEIS2, except the Program Normbeis3 reads only gridded landuse data that is in netCDF. The Biogenic Emissions Landcover Database version 3 (BELD3) is the typical database used for generating the gridded landuse files that go into Normbeis3. BELD3 consists of high-resolution (1-km horizontal resolution) land use data for 230 different land use types. BELD2 was the primary database used for BEIS2 applications. The Beld3to2 program can take the BELD3 data used in BEIS3 modeling and convert for use in BEIS2 modeling. It is also important to note that the GSPRO file used in Beis3 is not the same GSPRO file used in Tmpbio.

Mobile

The essence of mobile source emissions processing in SMOKE is converting link and county (also called, non-link) vehicle-miles traveled (VMT) data to hourly, gridded emissions of the chemical species used by an air quality model. In order to do this, SMOKE creates, manages, and applies MOBILE5b emissions factors to the VMT based on a user-defined definition of a "mobile control strategy". This control strategy can define the motor vehicle parameters either for a specific, historical year or for a hypothetical control strategy in the past, present, or future.

In SMOKE version 1.1, emissions data for mobile sources can also be imported into the system. In this case, the system knows not to try to generate emission factors. Emission factors are only generated for VMT data. The temporalization, gridding, and speciation are otherwise the same as when the emissions are generated using emission factors.

Raw input data

VMT data may be available as county-total and as link data, and SMOKE can use both. Links are straight road segments that by definition begin and end at coordinates that may not cross a county boundary. SMOKE contains is own line-grid intersection code to divide the link emissions into each grid cell.

Data can also be imported as emission values. In this case, the activity data such as VMT has already been combined with emission factors to get an emission estimate. When this processing option is selected, SMOKE does not manage the impact on emissions of the meteorological data, and this is instead left up to the user to implement (if needed) using temporal profiles or day-/hour-specific mobile data.

Currently, SMOKE permits the IDA and EMS-95 formats for nonlink data, a EMS-95-based list-directed format also for nonlink data, and a different list-directed format for link data. An upcoming version of Smkinven will permit gridded mobile data as input.

Emission factors created by MOBILE5b

Emission factors are created in SMOKE using MOBILE5b, for a wide variety of exhaust and evaporative processes and pollutants. Some of the MOBILE5b inputs parameters implement control strategies (e.g., inspection and maintenance (I/M) programs, anti-tampering programs (ATPs), and reformulated gas (RFG)). Other MOBILE5b inputs define other factors contributing to the value of the emissions factors, such as vehicle registrations (which help define the mix of different vehicle types), fuel volatility parameters, speeds, and temperature. All of these different dependencies make mobile emissions processing more complex than other types of sources.

Processing steps

In addition to importing the inventory and applying the emission factors, the remaining mobile

source processing steps are speciation, temporal allocation, projection of VMT, and gridding. These are implemented using the standard emissions cross-reference and profile approach in which each combination of county, road class, and link is indirectly assigned a profile number by using a cross-reference file. A given profile number is used to find the appropriate temporal profile, speciation profile, etc., that transform the raw data using factors from the profiles.

Sources

SMOKE mobile sources are defined in two groups: link and non-link. Both sources contribute vehicle-miles traveled (VMT) to the "mobile inventory". They are defined by the following attributes:

- Link sources: country, state, and county code; road type code, vehicle type code; Link ID; (X,Y) coordinates at the start of the link; (X,Y) coordinates at the end of the link
- Non-link sources: country, state, and county code; road type code, vehicle type code

A link is a straight road segment. Curved roads must be broken into several segments for proper spatial allocation. A GIS is typically used to perform link-source input preparation, but this activity is not integrated into SMOKE. Note that because the country/state/county code is part of the link-source definition, it is mandatory that the link coordinates not cross a county boundary.

Finally, the code used for identifying road type and vehicle type is imported into SMOKE as an SCC. In the 10-digit SCC, the final three digits are treated as the road type, and digits 3 through 6 are treated as vehicle type.

Temperature inputs

Because the MOBILE5b emission factors used by SMOKE are significantly influenced by temperature, the most desirable approach from an accuracy standpoint is to model mobile emissions using gridded, temporalized emissions from a meteorological model. However, in order to retain the performance benefits of source-based SMOKE processing, SMOKE has been designed to "ungrid" the temperatures to get a source-based temperature. For processing of all kinds, SMOKE expects one of the gridded, temporal temperature files MET_CRO_2D or MET_CRO_3D. The MET_CRO_2D file is used for surface or 1.5-meter temperature data. The MET_CRO_3D data file is used for ambient temperature data.

All of the emission factors depend on temperature in some way. The non-diurnal emission factors depend on a single temperature, which can be treated as a source-temperature for a given hour. They also depend on the minimum and maximum temperatures per day, which are treated as the minimum and maximum per source per day in SMOKE. The diurnal emission factors depend only on the minimum and maximum temperatures. SMOKE applies these temperatures to the source-based VMT using the minimum and maximum temperatures per source per day.

Temperature ungridding

SMOKE retains its performance benefits when processing mobile sources through the use of

"ungridded" temperatures. These temperatures are created by averaging the temperatures in the grid cells intersecting each mobile source, weighted by the fraction of the source's surrogate fractions (for non-link sources) or length (for link sources) intersecting those grid cells. The ungridding is implemented by building an "ungridding matrix," MUMAT, which must be created by the Grdmat program.

Parameter Scheme Index (PSI)

Each emission factor created, managed, and applied by SMOKE has an associated parameter scheme index (PSI). The PSI represents a unique combination of MOBILE inputs. The PSIs are defined in the MPREF file by associating a number with a MOBILE5b input file. These are call "pure" PSIs.

For example, one PSI could be used for all counties in a state with one type of inspection and maintenance (I/M) program, and another PSI for all counties without that I/M program. The counties without I/M programs would be assigned the PSI associated with the non-I/M MOBILE inputs, and the counties with I/M programs assigned the PSI associated with the I/M MOBILE inputs. The MOBILE inputs file, MPREF, associates the PSIs with the MOBILE inputs using the standard MOBILE input format, with header lines for assigning the PSIs. The simulation-specific emission factors cross-reference file (MPLIST) associates the PSIs (hence the emission factors) to the mobile sources. The PSIs in MPLIST must be a subset of the PSIs in MPREF.

Another kind of PSI, the combination PSI, can also be defined by referencing other PSIs and specifying multipliers for each. For example, PSI 005 could be calculated from 50 percent of PSI 003 and 50 percent of PSI 002.

Using PSIs provide significant benefits, including:

- permitting SMOKE to reduce the number of MOBILE5b runs for a given scenario,
- permitting SMOKE to reuse MOBILE5b emission factors between scenarios, and
- permitting the clear definitions of mobile control strategies for regional simulations.

Mobile control strategies

The PSIs facilitate the clear definition of control strategies. Such definition is important since SMOKE's speed creates the possibility of hundreds of mobile-source control strategies to be run. The components of a control strategy include all of the control features available in the MOBILE5b model, such as inspection and maintenance programs, anti-tampering programs, and reformulated gasoline. In addition, control strategies can be developed which explore the mixing of emission factors from different regions in a single region. For example, one could examine the impact of control programs in South Carolina and Georgia on interstate roads in North Carolina. The control strategy definition is in the file containing the PSI definitions for a given scenario.

Emission processes and emission types

Mobile SMOKE currently permits many, but not all, of the emissions-forming processes modeled in the MOBILE5b model used by SMOKE. The supported emission processes are the following.

- EXH: "exhaust" emissions for out-of-tailpipe contributions
- EVP: "evaporative" emissions processes. Note: EVP = HOT + CRC + WDL.
- RNL: "running loss" evaporative emissions from running vehicles not accounted for by other processes
- RST: "resting loss" evaporative emissions from resting vehicles, representing the time-period after the hot-soak is complete, but not associated with diurnal temperature variation.
- WDL: "weighted diurnal emissions" represent evaporative emissions from the carbon canisters (a control feature), that have been sitting for an assumed distribution of partial day, full day, and multiple day.
- DNL: "diurnal emissions" are evaporative emissions due entirely to diurnal variations in temperature, but in MOBILE5b depend only on the minimum and maximum temperatures during the day.
- HOT: "hot soak" emissions represent evaporative emissions occurring during the time a warmed-up engine has stopped running and is cooling down.
- CRC: "crankcase" emissions are evaporative emissions emanating from the crankcase of vehicles

Emission types are the combinations arising from combining the emission processes with each of the pollutants output by MOBILE5b, for example, EXH__NOX or EVP__VOC. Each emission type is associated with emission factors produced by the MOBILE5b emission factor model. Mobile SMOKE currently supports the following pollutants and process combinations that are output by MOBILE5b. Note that only one volatile component can be used at a time. In the example below, VOC could be replaced with any of the other volatile output pollutants available from MOBILE5b.

- EXH__CO (g/mi): Exhaust CO
- EXH__NOX (g/mi): Exhaust NO_X
- EXH__VOC (g/mi): Exhaust VOC
- EVP__VOC (g/mi): Evaporative VOC
- RNL__VOC (g/mi): Running VOC

- RST__VOC (g/mi): Resting VOC, by mile
- WDL__VOC (g/mi): Weighted diurnal VOC
- DNL__VOC (g/mi): Diurnal VOC
- HOT__VOC (g/trip): Hot soak evaporative VOC
- CRC__VOC (g/mi): Crankcase VOC

Because the EVP emissions are a sum of the WDL, HOT, and CRC emissions, it is not correct to use EVP and any of these three at the same time. Furthermore, since SMOKE does not yet permit input of trip information, using the HOT emission factor is incorrect as well. The recommended configuration encompasses the following emission types: EXH__CO, EXH__NOX, EXH__VOC, EVP__VOC, RNL__VOC, RST__VOC, DNL_VOC. The MEPROC file installed with SMOKE configures the system to be run in this way.

Road Classes

Descriptions of the road classes and their associated numeric codes are as follows. The AIRS AMS road class code is the same as the last three digits in the 10-digit SCC expected by SMOKE. Within SMOKE, the road class is stored as the combination of the area type code and facility type code. Other SMOKE inputs can use either the AIRS code or the area/facility code.

Name	AIRS AMS road class code	Area type code	Facility type code
Rural Interstate	110	0	1
Rural Principle Arterial	130	0	2
Rural Minor Arterial	150	0	6
Rural Major Collector	170	0	7
Rural Minor Collector	190	0	8
Rural Local	210	0	9
Urban Interstate	230	1	1
Urban Freeway	250	1	2
Urban Principle Arterial	270	1	4

Urban Minor Arterial	290	1	6
Urban Collector	310	1	7
Urban Local	330	1	9

Vehicle Types

The vehicle types used in on-road mobile source processing are described in the following table. The codes (e.g., 0100) should be used in the cross-reference files.

Code	Description
0100	LDGV: Light Duty Gasoline Vehicles
0102	LDGT1: Light Duty Gasoline Trucks 1
0104	LDGT2: Light Duty Gasoline Trucks 2
0107	HDGV: Heady Duty Gasoline Vehicles
3000	LDDV: Light Duty Diesel Vehicles
3006	LDDT: Light Duty Diesel Trucks
3007	HDDV: Heavy Duty Diesel Vehicles
0108	MC: Motorcycles

Internal SCCs

For mobile sources, SMOKE uses SCCs internal to the code to help with hierarchical matching by SCC during cross-referencing. While standard mobile SCCs have the structure vehicle-type // road-class, SMOKE needs the structure area-type // facility-type // vehicle type to use the appropriate hierarchies for emissions processing. For some readers of the mobile cross-reference files (e.g., temporal), errors and warnings may go to the log file that use the mobile internal SCCs.

Other Features

There are many other features for mobile source processing, which are documented in the SMOKE Core Programs Chapter. The relevant SMOKE programs are Smkinven, Spcmat,

Grdmat, Premobl, Emisfac, Temporal, Smkmerge, Grwinven, and Mrggrid. The various options for the SMOKE programs are usually applicable to mobile source emissions.

Point

The essence of point source emissions processing in SMOKE is converting inventory pollutant data for point source stacks from annual, daily, or hourly emissions to hourly and gridded emissions of the chemical species used by an air quality model. SMOKE processing may be performed either with or without control strategies. SMOKE accepts the raw data in two input formats: IDA and EMS-95.

Day-specific and hour-specific data

Emissions are often available as an annual total or daily average value. Emissions data are also sometimes available as day- or hour-specific totals. Smkinven can import the day- and hour-specific data, and it can also convert the hour-specific data to hour-specific temporal profiles. The SMOKE Temporal program is designed to accept these inputs and override the annual or daily emissions with the most specific data available.

Point sources are three-dimensional

Point source plumes may extend high into the vertical structure of the air quality modeling grid definition. For these elevated plumes, the plume rise needs to be modeled; the emissions from these sources must be provided to the air quality model in three dimensions (x, y, and z). The SMOKE prototype can model plume rise using two methods: the layer fraction method and the cutoff method, as described below.

Processing Steps

In addition to inventory import and plume rise, the remaining point source processing steps are speciation, temporal allocation, projection, control, and spatial allocation. These are implemented using the standard emissions cross-reference and profile approach in which each county, SCC code, plant ID, and stack ID is indirectly assigned a profile number by using a cross-reference file. A given profile number is used to find the appropriate temporal profile, speciation profile, etc., that transforms the raw data using factors from the profiles.

Sources

Depending on the input format of point source emissions, the unique set of characteristics (or *keys*) that are used to uniquely identify a point source is different. For example, the Emissions Preprocessing System 2.0 (EPS2.0) defines a point source using a country, state, and county code, a SCC, a plant identifier, a stack number, a point identifier, and a segment number. The Emissions Modeling System, 95 (EMS-95), however, identifies a source using a FIPS state/county code, a plant code, a stack code, a device code, and a process code. Also, the National Emission Trends (NET) format has yet another definition of point sources. To better

support all of these formats, SMOKE has been updated to permit a flexible definition of point sources. This definition now consists of the following keys:

- Country, state, and county code
- Plant ID (15 characters or less)
- Characteristics 1 through 5 (all 15 characters or less)

Depending on the input format, SMOKE assigns different variables from the input format to the fields of the SMOKE point source definition. The source characteristics for a given inventory type need to be considered when cross-reference files are created.

Layer fraction method

SMOKE has two distinct methods for calculating plume rise, one of which must be selected for use in processing. This decision is based on the air quality model for which the emissions are being prepared. The MAQSIP and CMAQ models require the layer fraction method, because these models typically have fine vertical resolutions. For this method, meteorological data are used to calculate the plume rise for all point source emissions using essentially the same method as in the RADM air quality model. Then, the plume is evenly distributed into the vertical layers that the plume intersects. Only these fractions are stored (not the emissions in each layer), until the SMOKE merge step. Consequently, the plume rise calculations do not need to be repeated for each control strategy or grid (unlike the situation in which the plume rise calculations are done inside the air quality model, such as in the UAM-IV and UAM-V). The plume rise is calculated using the Laypoint program for all days of each meteorological scenario.

Cutoff method

Another approach to modeling plume rise is first to quickly estimate the plume rise using a Briggs-algorithm plume rise calculation similar to that found in EPS2.0, and then to compare this plume rise to a user-defined cutoff value. Sources below this cutoff value are treated as single-layer point sources, and sources above this cutoff are considered elevated point sources. In SMOKE, the Elevpoint program makes this distinction. The Temporal program then outputs separate hourly-emissions files for single-layer and elevated point sources. UAM-IV, UAM-V, and CAMx use these files. The Briggs algorithm is provided with the documentation to the Elevpoint program.

Multiple year-to-year projections

SMOKE can combine raw data from different inventory years into a single inventory. The inventory year is stored as one of the records in the SMOKE point source inventory file PNTS. The data from these different years can then be projected to the same year using the Cntlmat projection and controls program. The format of the projection data in this file has been designed so that the projection factors are listed with the "from year" and the "to year".

Other Features

There are many other features for mobile source processing, which are documented in the SMOKE Core Programs Chapter. The relevant SMOKE programs are Smkinven, Spcmat, Grdmat, Elevpoint, Temporal, Laypoint, Smkmerge, Grwinven, and Mrggrid.
