Emissions Modeling

Marc Houyoux, U.S. EPA,
Houyoux.marc@epa.gov

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Part 1:
Emissions Modeling Concepts

Emissions Modeling Concepts

- **Source categories**
- **Definitions**
- **Nonpoint emissions processing**
- **Point emissions processing**
- **Mobile emissions processing**
- **Biogenic emissions processing**
- **Merging**
- **Quality assurance**
- **Getting started with SMOKE**

Source Categories (1)

- **Non-point (area) and nonroad mobile source characteristics**
  - **Country, state, county**
  - **Source category code (SCC)**
- **Point source characteristics**
  - **Country, state, county, and…**
  - **Plant, point, stack, segment, SCC, for…**
    - **National Inventory Format (NIF)**
    - **National Emission Inventory (NEI) in Inventory Data Analyzer (IDA) format**
    - **Emissions Preprocessing System input format**

Source Categories (2)

- **On-road mobile source characteristics**
  - **Country, state, county**
  - **Road type (e.g., rural interstate, urban local)**
  - **Vehicle type (e.g., light duty gasoline vehicles)**
  - **Link ID (optional)**
- **Biogenic source characteristics**
  - **Country, state, county**
  - **Landuse type**
    - **OR**
  - **Grid cell**
  - **Landuse type**

Definitions (1)

- **<u>Inventory pollutant</u>: A compound or group of compounds defined for record-keeping and regulatory purposes (e.g. CO, NO_x, VOC, PM_{10})**

- **<u>Species</u>: A compound or group of compounds defined as part of the estimation of air chemistry in an air quality model (e.g., CO, NO, NO_2, PAR, ECC)**

- **<u>Chemical mechanism</u>: A set of chemical species and their interactions used to represent air chemistry (e.g., CB-IV, RADM, SAPRC)**
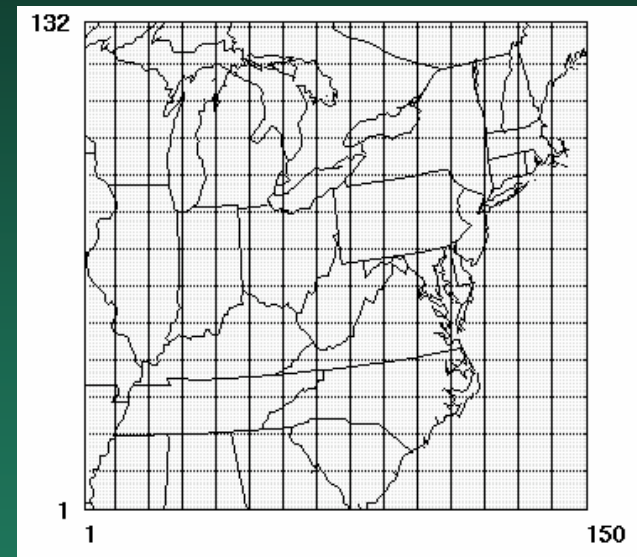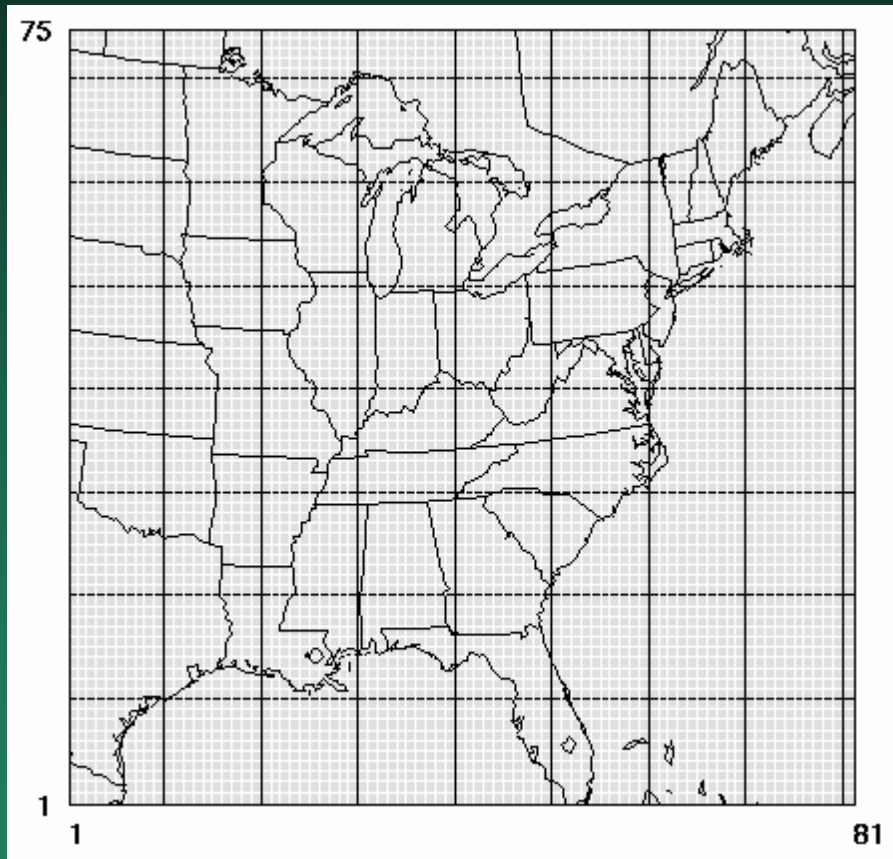
Definitions (2)

- <u>**Map projection**</u>**: The mathematical representation of the spherical surface of the earth in 2-d**

- <u>**Model grid**</u>**: A 2-d grid based on a map projection, defined by starting coordinates, number of grid cells in each direction, and the physical size of the grid cells**

Examples of Model Grids

Definitions (3)

- **Model layers: Vertical spatial divisions defined by an air quality model because the atmosphere has varied characteristics in the vertical direction**

- **Plume rise: The rising of the exhaust from point sources due to the velocity and temperature of the exhaust gases**

- **Elevated source: A point source in which emissions are higher than the first model layer because of plume rise**
  - **Note: This definition is often different from that used for UAM-based air quality models**

- **Plume-in-grid: A special treatment of elevated sources by which the plume rise is modeled with extra detail by the air quality model**

Definitions (4)

- **<u>Spatial allocation</u>:** Convert the source spatial extent to the grid cell resolution (or census track) needed by the air quality model

- **<u>Chemical speciation</u>:** Convert the inventory pollutant data to the chemical species needed by the air quality model (e.g., VOC gets split to PAR, OLE, XYL, TOL, ISOP, and more).

- **<u>Temporal allocation</u>:** Convert the inventory temporal resolution to the temporal resolution needed by the air quality model (e.g., month/day-specific hourly, 3-hour)

Definitions (5)

- **Emissions Projection: converting emissions from one year to emissions from another year using growth and control factors.**

- **Growth factors: The estimated increase (or decrease) in emissions from one year to another year. Typically used to estimate future-year emissions based on the assumption that economic growth by SIC or SCC represents emissions changes.**

- **Control factors: Emissions reduction factors to account for control programs from one year to another year. Used with inventory control information typically to estimate future-year emissions.**

Definitions (6)

- **<u>Profile data</u>: Factors used for disaggregating emissions data as is done during chemical speciation or temporal allocation**

- **<u>Cross-reference</u>: A dataset used for matching sources in the emissions inventory with profile data based on the source characteristics**

- **<u>Gridding surrogate</u>: A dataset developed from data at a finer resolution than the emissions, used to spatially allocate the emissions to the grid cells (e.g., population, housing, agricultural regions)**
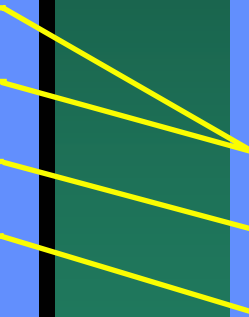
Definitions (7)

Cross-references and profiles or surrogates:

X-REF table	Profiles table

State, County, ID	ID, Factor 1, 2, 3
NC, Durham , 15	13 0.2, 0.3, 0.5
NC, Orange, 15	14 0.4, 0.4, 0.2
NC, Wake, 16	15 0.4, 0.3, 0.3
SC, All 17	16 0.4, 0.5, 0.1
	17 0.4, 0.4, 0.2

Nonpoint Emissions Processing

- **Import data**
- **Spatial allocation**
  - **Allocation of county emissions into grid cells using spatial surrogate**
  - **Distribute county-total emissions nonuniformly to grid cells that intersect the county based on variation of some other dataset (I.e., a "surrogate" data set)**
- **Chemical speciation**
- **Temporal allocation**
- **Growth and control for future year**
- **This approach also applied for vehicular road dust and nonroad mobile sources**

Point Emissions Processing

- **Import, chemical speciation, temporal, growth/control plus...**
- **All emissions for a source in single grid cell**
- **May use day-specific and hour-specific emissions**
- **Determine elevated sources and plume-in-grid (PinG) sources**
- **Special processing and output for elevated and PinG sources**
  - **Create meteorology-based 3-d emissions file & optional PinG emissions files for CMAQ or MAQSIP**

    OR
  - **Create special elevated (PinG optional) & 2-d emissions file for UAM-based models**

On-road Mobile Emissions Processing (1)

- **Steps for nonpoint sources, plus...**

- **Possibly start with vehicle miles traveled (VMT) instead of emissions**

- **Create emission factors based on meteorology**
  - **Emission factors model such as MOBILE5b or MOBILE6**
  - **Gridded hourly or average meteorology**
  - **Emissions = Emission factor $\times$ VMT**

- **Spatial allocation may include link sources (i.e., sources with VMT assigned to a line source within a county)**

On-road Mobile Emissions Processing (2)

- **Emission factors typically depend on emissions process (e.g., start exhaust, running exhaust, evaporative, diurnal evaporative)**

- **Temporal allocation and chemical speciation can depend on emissions process**

- **Approach only for on-road mobile sources (nonroad mobile and vehicular road dust processed as nonpoint sources)**

Biogenic Emissions Processing

- **Typically created by BEIS2 or BEIS3 emissions model or derivative**

- **About 230 landuse types (for BELD3 data)**

- **Landuse types have emission factors which are adjusted by gridded temperature and solar radiation**

- **Winter and summer emission factors**

- **If landuse is county total, then use gridding surrogate to allocate emissions to grid cells**

- **Plants and soil emissions, not geogenic**

Merging and Formatting

- **Combining steps taken for a given source category to create model-ready formatted files (e.g., combine import, gridding, speciation, temporal allocation steps)**

- **Combine multiple source categories into a single data set (e.g., combine area, biogenic, mobile, and point)**

- **Output correct units, species, time steps, grid, and file format for the air quality model of interest**

Quality Assurance

- **Compare emissions totals from emissions processor with inventory totals**
  - **By state, county, SCC, combinations, other**
- **Compare emissions totals at each stage of the processing. Ensure most applicable profiles & surrogates.**
- **Ensure input file formats are correct**
- **Ensure no significant errors or warnings in processing**
- **Compare emissions among states and counties**
- **Compare emission ratios to ambient measurement ratios**
- **Compare current run to previous runs**

Available Emissions Models

- **EPS2.0 and EPS2.5 – Fortran based tool used to prepare inputs for REMSAD and CAMx models.**

- **EMS-2000 – SAS based tool used to prepare inputs for CAMx, CMAQ, and perhaps others.**

- **CONCEPT – New RPO-developed tool based on PostgreSQL freeware database initial stages of release to prepare inputs for CAMx, CMAQ, perhaps others**

- **SMOKE – Fortran and UNIX/Linux scripts-based tool to prepare inputs for REMSAD, CAMx, CMAQ (including Hg and toxics versions).**

New EmisView QA Tool

- **Tabular and graphical emissions modeling QA tool**
- **Integrated with SMOKE and CONCEPT, limited functions with EPS**
- **Open source and free**
- **Written in Java so can run on Windows and UNIX/Linux**
- **Schedule**
  - **Version available for demo at conference**
  - **Public beta version soon (1 week?) after conference**
  - **Updated version with more capabilities by August, 2005**
  - **Additional updates in late 2005, early 2006**
- **http://emisview.sourceforge.net/**

Getting Started with SMOKE

- **Capabilities (three slides)**
- **Dataflows (four slides)**
- **Upcoming SMOKE-related updates**
- **Other emissions modeling-related happenings at EPA**

SMOKE Capabilities (1)

- **Process criteria and toxics inventories**
- **Can integrate toxics and criteria to prevent double counting of VOCs**
- **Imports ASCII formats, not NIF:**
  - **Inventory Data Analyzer (IDA)**
  - **One-record-per-line (ORL) primarily for toxics**
  - **EMS-95**
- **Spatial allocation for nonpoint and on-road mobile with spatial surrogates and point based on lat/lon or UTM coordinates.**

SMOKE Capabilities (2)

- **CB-IV, RADM, SAPRC, CB-IV toxics for CMAQ mechanisms installed by default, including particulate splits**

- **Aggregation and disaggregation of toxic compounds**

- **Supports monthly, weekly, and diurnal profiles**
  - **Different diurnal permitted for each day of the week**

- **Can use ozone-season or annual-average inventory data from IDA and toxics inventories**

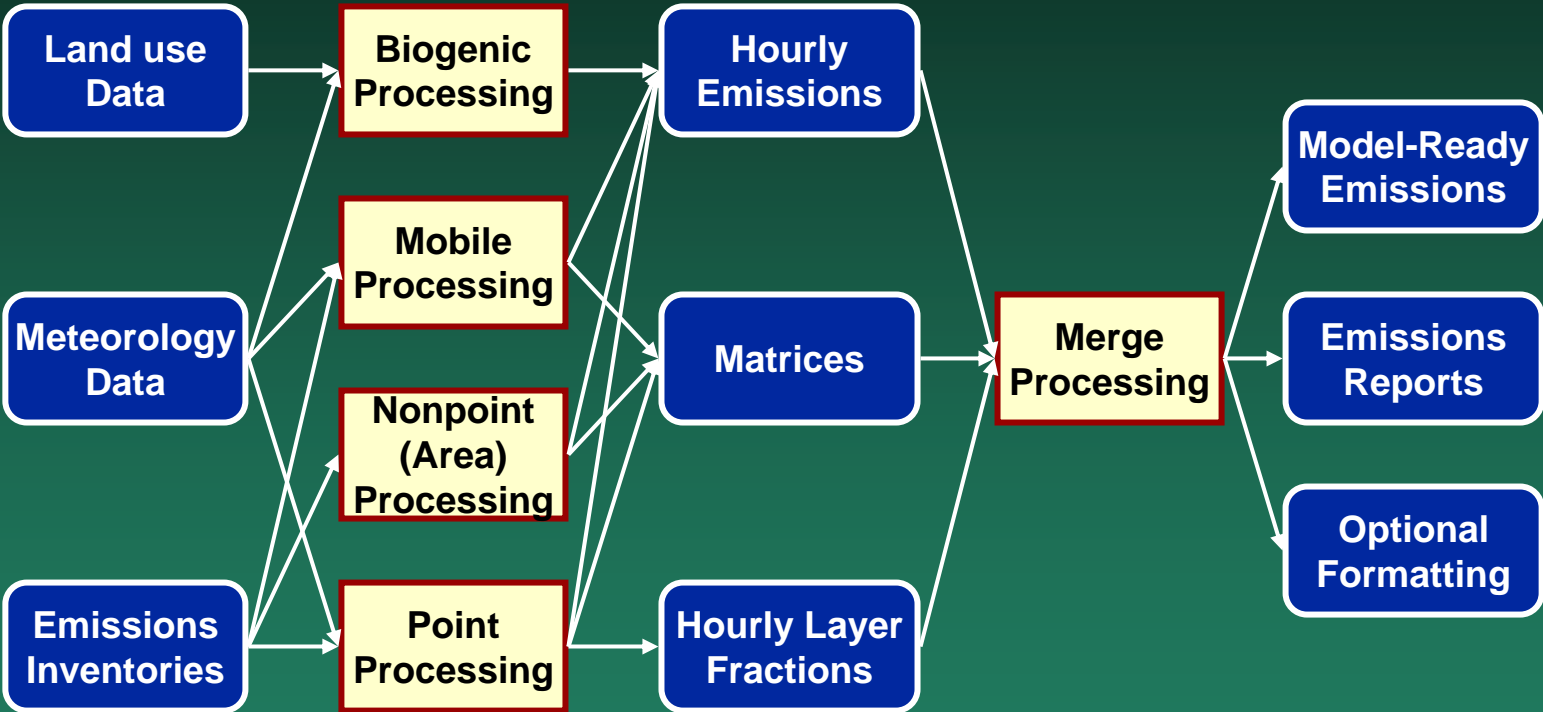- **Grow and control point, nonpoint, nonroad mobile, on-road mobile.**
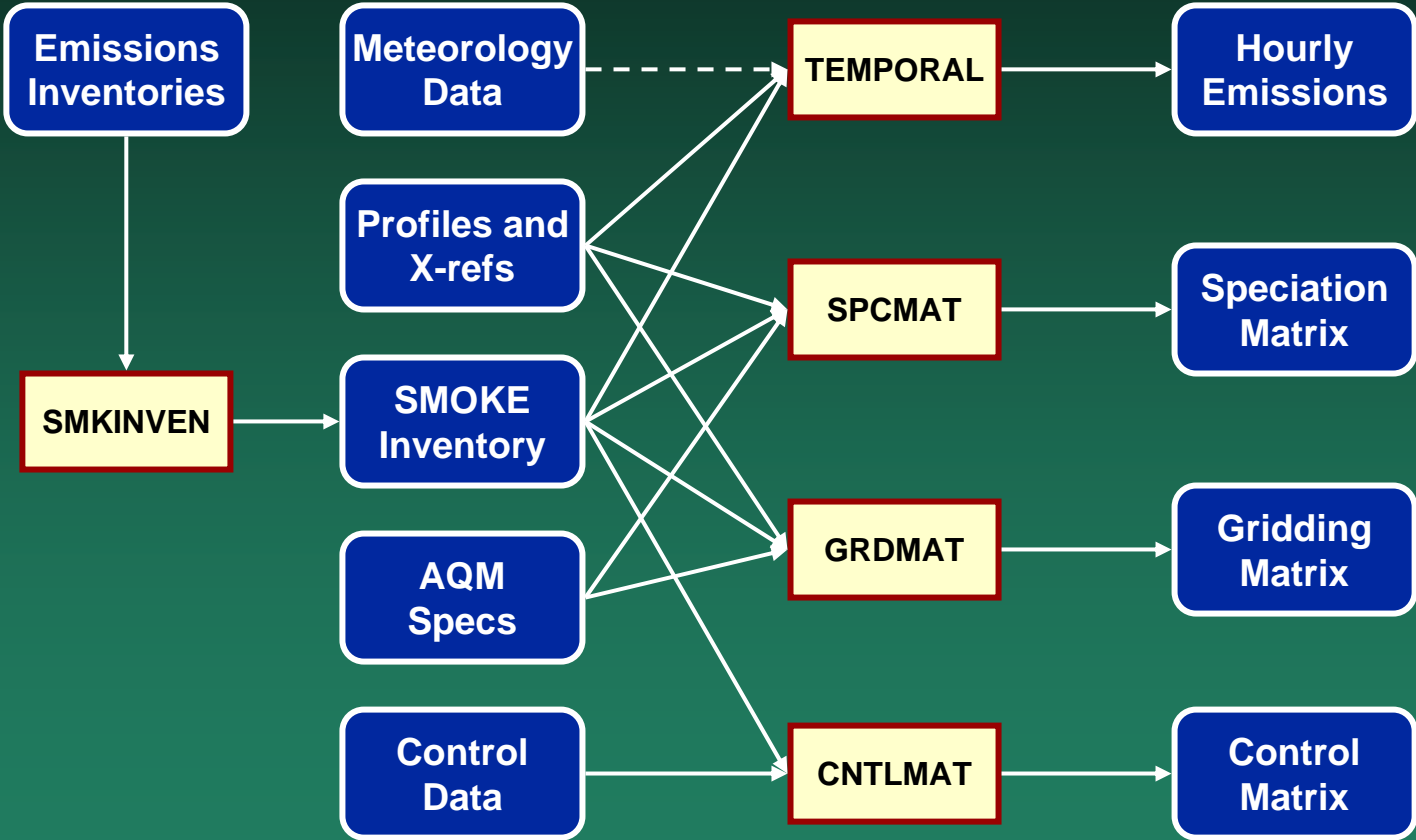
SMOKE Capabilities (3)

- **On-road mobile optionally drives MOBILE6 for meteorology-dependent emissions calculations**
- **Biogenic emissions with BEIS2 or BEIS3**
- **Compute point source plume rise when needed (i.e., CMAQ) and identify elevated sources by stack parameters or plume rise**
- **Output for CMAQ, REMSAD, CAM_X, MAQSIP, UAM**
- **ASCII summaries for quality assurance and post-processing**

SMOKE Dataflows (1)

SMOKE Dataflows (2)

Other Processing Paradigms

| Load Inventory | → | Growth and Controls | → | Speciation | → | Temporal Allocation | → | Gridding | → | Model Ready Emissions |

SMOKE Processing Paradigm

Load Inventory →
- Temporal Allocation
- Growth and Controls
- Speciation
- Gridding

→ Merge → Model Ready Emissions
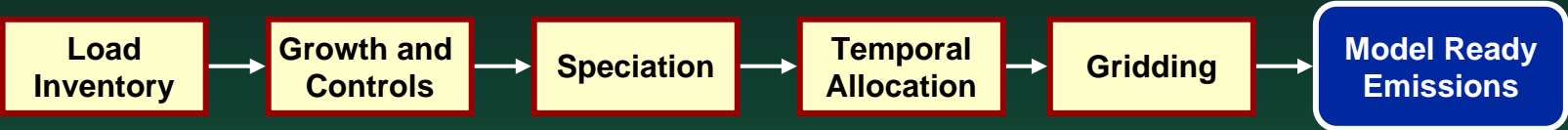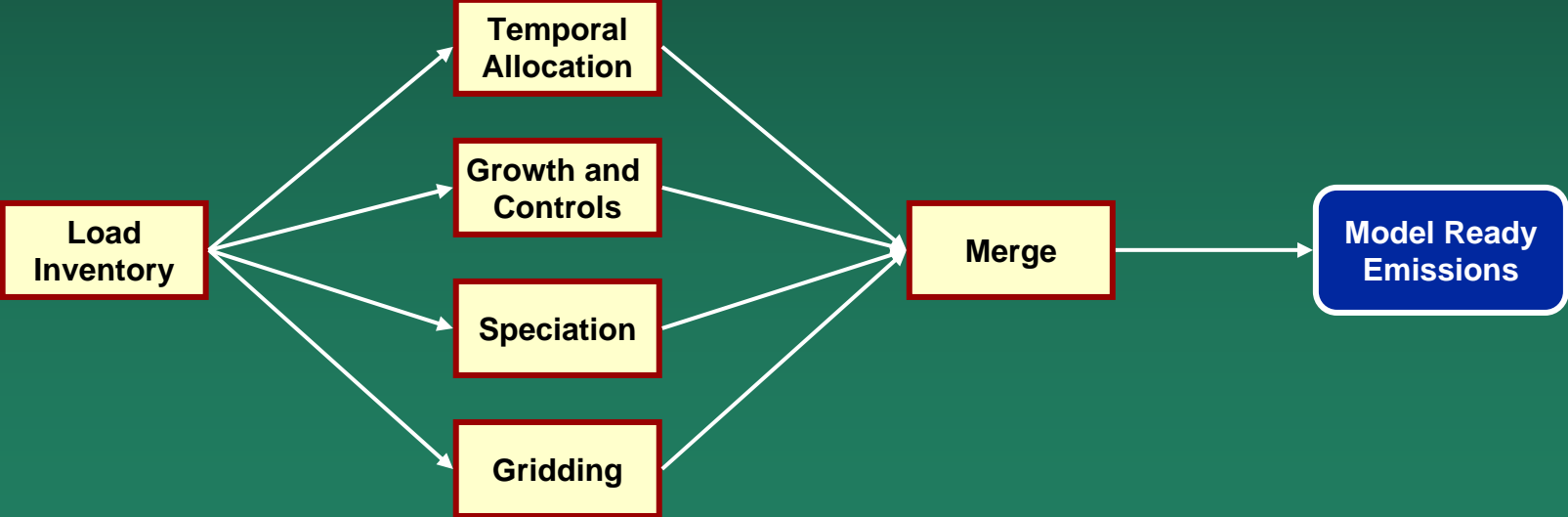
SMOKE for Additional Control Strategies

Growth and Controls → Merge → **Model Ready Emissions**

SMOKE for Additional Grids
(for sources that do not use VMT)

Gridding → Merge → **Model Ready Emissions**

SMOKE for Additional Grids
(for mobile sources that do use VMT)

Gridding → Emission Factors → Temporal Allocation → Merge → **Model Ready Emissions**

Upcoming SMOKE changes (1)

- **EPA developing Emissions Modeling Framework to provide:**
  - **Database-based data management functions (by end of 2005):**
    - **Data versioning and change tracking**
    - **Multi-user emissions modeling tool for sharing work within an organization**
    - **Data change notification**
    - **Integrated user-defined QA protocols on new data**
    - **Data problem tracking**
  - **SMOKE GUI for setting up and running SMOKE programs (by June 2006)**
  - **Model run management for handling multiple jobs at the same time on (possibly) different computers and/or on cluster**

Upcoming SMOKE changes (2)

- **Full support for ASPEN model (toxics)**
- **Improvements for using hourly CEM data**
- **New approaches for fire data**
- **Improved approaches for growth and control**
- **Additional QA functions**
- **Generating spatial surrogates using the MIMS Spatial Allocator**
- **Generating speciation profiles, including CMAQ for toxics**
- **These and others planned for completion and release by this September.**

Other Emissions Modeling Happenings at EPA

- **SPECIATE4.0 likely to be released this year (Lee Beck)**
- **Additional EGAS5 updates (Aaiysha Kursheed)**
- **New version of AirControlNET (Larry Sorrels)**
- **Trying to get a national control programs database, but funding sources not yet identified**
- **2002 final NEI planned for release in December (Doug Solomon)**
- **Comparison of 2002 NEI and RPO 2002 inventories (Doug Solomon)**
- **National Mobile Inventory Model, NMIM (Harvey Michaels)**
- **MOVES model (Megan Beardsley)**
- **2002 NATA modeling (Madeleine Strum)**

Part 2:
EPA's Latest Modeling Inputs:

Emissions Data used for the
Clean Air Interstate Rule (CAIR)
and the
Clean Air Mercury Rule (CAMR)

EPA Emissions Modeling Files

- **Overview**
- **Additional information availability**
- **1999/2001 inventories**
- **Miscellaneous ancillary files**
- **Temporal allocation**
- **Spatial allocation**
- **Chemical speciation**
  - **CMAQ CB-IV with PM**
  - **REMSAD7 (not used for CAIR or CAMR)**
  - **Mercury**

Overview

- **Two major types of emissions modeling inputs: inventory files and ancillary files**

- **Inventory files contain the emissions and VMT**

- **Ancillary files are everything but the files that contain the emissions and handle:**
  - **Providing names that are not included in the raw inventories (e.g. for country, state, and county codes, SCCs)**
  - **Applying factors for temporal, spatial, and chemical allocation of emissions**
  - **Factors for growth and controls**
  - **Controlling reporting**

- **This class will use SMOKE input files as examples, though some of the files can be used in other modeling systems.**

Detailed documentation available

- **CAIR Technical Support Document:**
  www.epa.gov/air/interstateairquality/pdfs/finaltech01.pdf

- **CAMR Technical Support Document:**
  www.epa.gov/ttn/atw/utility/emiss_inv_oar-2002-0056-6129.pdf

Data files available

- **Additional data available, but not provided with training:**
  - Growth and control factors for non-EGU and stationary area sources
  - All months for on-road and nonroad mobile data
  - 2001, 2010, 2015, and 2020 VMT data
  - 2010, 2015, and 2020 criteria emissions in SMOKE input format
  - 2020 Hg emissions in SMOKE input format
- **CAIR and CAMR data available in EPA's "docket"**
- **Easier way to get it on OAQPS ftp site**
  - Contact Warren Peters at peters.warren@epa.gov for password
  - CAIR: ftp://airmodelingftp.com/cair_noda/cair_noda/emissions/
  - CAMR: ftp://airmodelingftp.com/CAMR

Emission Inventory Group

2001 Criteria for CAIR
Overview

- **All 2001 files are in SMOKE's IDA format defined in SMOKE manual (a text format)**

  http://www.cep.unc.edu/empd/products/smoke/version2/ ch08_input_files.pdf

- **Contain CO, NOx, VOC, NH3, SO2, PM2.5, PM10**

- **PM emissions include condensibles where possible**

- **Zip file of data files available online at:**

  http://www.epa.gov/ttn/chief/emch/invent/index.html#smoke

1999 Mercury for CAMR

- **U.S. Inventory files are in SMOKE's ORL format defined in SMOKE manual (a text format).**

- **Canadian inventory files in SMOKE IDA format**

- **Contain a combination of pre-speciated (PHGI, HGIIGAS, HG) and unspeciated (HGSUM) mercury data**

- **Zip file of data files available online at:**
  http://www.epa.gov/ttn/chief/emch/invent/index.html#smoke

Base Point data files (1)

- ## Point sources (criteria and Hg)
  - ### Separated into EGU and nonEGU inventories by identifying facilities modeled by the Integrated Planning Model (IPM).
  - ### Criteria separated point-source fugitive dust emissions into separate category
  - ### Stack parameters coordinated between 2001 criteria, 1999 Hg, and future-year inventory files
- ## All 2001 criteria data based on 2001 NEI (1999 NEI version 3 grown to 2001) with minor changes

Base Point data files (2)

- **Important information:**
  - **Fugitive dust file needs application of transportable fractions**
  - **Data in "IPM" file not calculated by IPM – simply the sources**
  - **Not all IPM facilities matched – there is a different universe of facilities in IPM than in the NEI. Little coordination is done leading to facilities missing from the NEI and closed facilities in IPM.**
  - **Different source identifiers (e.g., plant IDs) in criteria and Hg datasets, but EPA has a mapping available.**
  - **ptnonipm changes from 1999 NEI documented in CAMR TSD**

Review point source inventory files and format

- **EGUs (IPM facilities):**
  inventory/ptipm/EGU_01v3_031211.emis.mod20040319
  inventory/hg_ptipm/Hg_99_2001_IPM.orl_mod03Dec2004

- **nonEGUs:**
  inventory/ptnonipm/negu_01v3_031211.emis.mod20040316

- **Fugitive dust:**
  inventory/pfdust/pt_fug_01v3_031211.emis

IDA file headers

- **Header lines always start with # sign in column 1**
- **#IDA always needs to be on line 1**
- **#TYPE sets the SMOKE file type (critical to get the correct name only for on-road mobile and toxics ORL files)**
- **#COUNTRY sets the country (SMOKE by default supports countries US, CANADA, MEXICO and others)**
- **#YEAR sets the inventory year**
- **#DATA sets the names and order of emissions data variables in the file (alt. #POLID)**
- **#DESC used for unlimited descriptive text**

ORL file headers

- **Same as IDA except:**
- **#ORL is always on the first line**
- **No #DATA header: the pollutants are defined separately on each line of the file using a CAS number, which assigns pollutant names by the SMOKE "inventory table" file**

Base Nonpoint stationary data files (1)

- **Nonpoint stationary sources (criteria and Hg)**
  - **Criteria separated into fugitive dust, agricultural NH3 (livestock and fertilizer), fires (wildfires, prescribed burning, agricultural burning, and open burning), and "other area"**
  - **Fires available as "average fires" or 2001-specific**
  - **Hg data just for single nonpoint sector**
- **Fugitive dust, fires, and "other" based on 2001 NEI. 2001 commercial cooking replaced with 2002 "preliminary" commercial cooking for completeness.**
- **Agricultural livestock based on new 2002 approach on EFIG 2002 NEI website and fertilizer based on 2001 NEI**

Nonpoint stationary data files (2)

- **Important information:**
  - **Fugitive dust file needs application of transportable fractions**
  - **Average fires approach:**
    - **Only wildfires and prescribed burning are averaged – ag burning and open burning are still 2001 estimates**
    - **2001 county-level fires * (1996-2002 state acres burned / 2001 state acres burned)**
  - **Livestock NH3 does not require the across-the-board 30% reduction.**
  - **Minor nonpoint Hg changes from 1999 NEI documented in CAMR TSD**

Emission Inventory Group

Review nonpoint source inventory files and format (1)

- **Fugitive dust:**
  inventory/afdust/idafug01_roaddust_121103.txt

- **Agricultural NH3:**
  inventory/ag/ar_fert_01v3_031212.emis
  inventory/ag/BeefNH3_IDAfmt.012304.txt
  inventory/ag/DairyNH3_IDAfmt.012304.txt
  inventory/ag/Horses-Goats-SheepNH3_IDAfmt.012304.txt
  inventory/ag/PoultryNH3_IDAfmt.012304.txt
  inventory/ag/SwineNH3_IDAfmt.012304.txt

- **Fires:**
  inventory/fire/ar_fire_01v3_031212.emis

Review nonpoint source inventory files and format (2)

- **Average fires:**
  inventory/avefire/arinv.fire_us_ave_1996-2002.ida

- **Other area sources:**
  inventory/oarea/ar_other_01v3_031218.emis_mod040309
  inventory/oarea/arinv.airport_refueling.01v3_031218.ida
  inventory/oarea/arinv.onroad_refueling.01v3_031218.ida
  inventory/oarea/ComCooking2002_ida_120403.txt

- **Hg nonpoint sources:**
  inventory/hg_nonpt/nonpoint99_hgESD_111804_noMWI_boilersfixed.orl

Mobile data files

- **Mobile sources (criteria only)**
  - **Separated into nonroad and on-road**
- **Both created by NMIM on a month-specific basis except for commercial marine, locomotives, and airports.**
- **California annual emissions used instead of NMIM results**
- **Important information:**
  - **Using county-total emissions by SCC per month**
  - **Monthly variation is temperatures (one or two monthly average temperatures per state), fuel information, control programs, etc. as reflected in this version of the NMIM database**
  - **For NMIM-based files, annual emissions fields not filled in (only average-day fields)**
  - **Locomotives and airports from 2001 NEI**
  - **Commercial marine from OTAQ national number scaled to counties using 2001 NEI.**

Review mobile source inventory files and formats

- **Nonroad files (NMIM files January only):**
  inventory/nonroad/arinv_nr_2001_jan_09mar04.emis
  inventory/nonroad/nr_01v3_040304_airport.ida
  inventory/nonroad/nr_01v3_040308_trains.ida_mod040311
  inventory/nonroad/nr_01v3-OTAQblend_040309_cmv.ida

- **On-road files (NMIM files January only):**
  inventory/mobile/mbinv_2001_jan_29mar04.emis_mod12apr04
  inventory/mobile/mbinv_ca_st_2001_ann2.emis

Miscellaneous ancillary files (1)

- **County-specific transportable fractions**
  - **Used to adjust the fugitive dust emissions in the inventory to reflect emissions that do not settle quickly**
  - **In SMOKE, done using same-year projection packet**
  - **File: inventory/afdust/gcntl.xportfrac.txt**
- **Country, state, and county file**
  - **Assign names to country, state, and county codes for reporting**
  - **Defines the valid country, state, and county codes**
  - **Defines time zones and daylight savings time by county**
  - **Contains county bounding boxes and centroids (not currently used by SMOKE)**
  - **File: ge_dat/costcy.txt**
- **Inventory file**
  - **Defines names and information by CAS number for ORL format**
  - **File inventory/other/invtable.hgonly.txt**

Emission Inventory Group

Miscellaneous ancillary files (2)

- ## SCC description file
  - Sets SCC descriptions for reporting (In SMOKE, these can appear in the Smkreport output reports)
  - File: ge_dat/scc_desc_030804.txt

- ## Surrogates description file
  - Defines the spatial surrogate codes in the spatial surrogates file
  - Would be better to have in header of spatial surrogates file
  - File: ge_dat/srg_desc_EPA1999.txt

- ## SIC description file
  - Sets SIC descriptions for reporting
  - File: ge_dat/sic_desc.txt

Temporal allocation (1)

- **Temporal profiles, cross-reference, & holiday files**
- **CAIR data available in SMOKE input and Excel on website: http://www.epa.gov/ttn/chief/emch/temporal/index.html**
- **Important information**
  - **Most content of these files has been taken from default file on EFIG website, without much review by EPA: http://www.epa.gov/ttn/chief/emch/temporal/**
  - **Diurnal and weekly profiles for on-road mobile based on NC data applied nationally**
  - **Contains WRAP wildfire diurnal profile**
  - **CAMR EGUs used a different temporal cross-reference file to improve consistency in temporal allocation between base and future years arising because of SCC changes.**

Temporal allocation (2)

- **Have added the following data:**
  - **State- and year-specific monthly profiles for wildfires, prescribed burning, ag fires (VISTAS states only), and open burning (VISTAS states only) for 1999 through 2002**
  - **New average-year monthly profiles are available for fires as well**
  - **State-specific diurnal profiles for wildfires and prescribed burning**
  - **State-specific fertilizer monthly profiles from CMU model**
  - **State-specific dairy cow monthly profiles from CMU model calculated by using a weighted average of county-specific CMU profiles using 2002 dairy cow county emissions**
  - **"Gilliland" profile for other livestock sectors based on inverse AQ modeling – normalized to not include a 30% reduction factor as it did originally**
  - **California-specific on-road monthly profiles by pollutant based on NMIM results, to add temporal variation to the California-supplied annual on-road emissions.**
  - **Made-up diurnal profile for commercial cooking.**

Cross-referencing simplified:

X-REF table   **Profiles table**

State, County, ID		ID, Factor 1, 2, 3
NC, Durham , 15		13 0.2, 0.3, 0.5
NC, Orange, 15		14 0.4, 0.4, 0.2
NC, Wake, 16		15 0.4, 0.3, 0.3
SC, All 17		16 0.4, 0.5, 0.1
		17 0.4, 0.4, 0.2

Review temporal allocation files and formats

- **Temporal cross-reference files:**
  ge_dat/amptref.m3.us+can.txt (CAIR)
  ge_dat/amptref.m3.avefire.us+can.txt (CAIR)
  ge_dat/ptref.hg_ptipm.txt (CAMR)

- **Temporal profile files:**
  ge_dat/amptpro.m3.1999.us+can.txt
  ge_dat/amptpro.m3.2000.us+can.txt
  ge_dat/amptpro.m3.2001.us+can.txt
  ge_dat/amptpro.m3.2002.us+can.txt
  ge_dat/amptpro.m3.default.us+can.txt

- **Holiday file:**
  ge_dat/holidays.txt

Spatial allocation (1)

- ● **Spatial surrogates, cross-reference available at**

  http://www.epa.gov/ttn/chief/emch/spatial/newsurrogate.html

- ● **Grid definition defines map projection and grid**

- ● **Important information**

  - ● **Web site has 4km, 12km, and 36km spatial surrogates for the U.S. and Canada. GIS shape files are available as well.**

  - ● **Canadian surrogates not as extensive or well quality assured.**

  - ● **A methodology has been used to "fill in" surrogates with other surrogates for all counties using the next best surrogate. The documentation for this is available on the website.**

  - ● **A Mexican surrogate section has been added, though only the population surrogate is being used by the cross-reference. The Mexican surrogates have not been well QA'd.**

Review spatial allocation files and formats

- **Spatial cross-reference file:**
  ge_dat/amgref.m3.us+can+mex.txt

- **36-km spatial surrogate file:**
  ge_dat/abmgpro.us+can+mex.us36b.txt

- **Grid definition file:**
  ge_dat/GRIDDESC

Chemical speciation – CMAQ (1)

- **Speciation profile, cross-reference file, and VOC-to-TOG conversion file**
- **Important information**
  - **Speciation profiles for VOC and PM2.5 from EPA web site http://www.epa.gov/ttn/chief/emch/speciation/**
  - **PM2.5 profiles have been updated for agricultural burning, coal combustion, paved road dust, wildfires, and wood waste boilers.**
  - **Updates for BEIS3.09 and BEIS3.12 modeling speciation**
- **Criteria modeling files (CAIR and CAMR):**
  Cross-ref file: ge_dat/gsref.cmaq.cb4p25.txt
  Profile file: ge_dat/gspro.cmaq.cb4p25.txt
  VOC-to-TOG: ge_dat/gscnv.txt

Chemical speciation – CMAQ (2)

● **Mercury modeling files (CAMR only):**

Cross-ref file:	**ge_dat/gsref.cmaq.cb4tx1p25.txt**
Profile file:	**ge_dat/gspro.cmaq.cb4tx1p25.txt**

Chemical speciation – REMSAD7

- **Speciation profile and cross-reference file**
- **NOT used for CAIR or CAMR**
- **Important information**
  - **No VOC profiles (REMSAD does need speciated VOC)**
  - **No VOC-to-TOG file for same reason**
  - **Same PM2.5 profiles and updates**
  - **XYL and TOL "profiles" add mass to the REMSAD inputs, and these species are used for estimating secondary organic aerosols.**
- **Cross-ref file:**   ge_dat/gsref.remsad7.cb4mpm.txt
  Profile file: ge_dat/gspro.remsad7.cb4mpm.txt

Default stack parameters

- **Stack-parameter defaults (height, diameter, exit temperature, and exit velocity)**

- **Used in case of missing stack parameters in the inventory file**

- **Assigns stack parameters by SCC**

- **In SMOKE, only those parameters that are missing are replaced with these, which can lead to inconsistencies. Better to correct the missing stack parameters in the inventory.**

- **File: ge_dat/pstk.m3.txt**

Emission Inventory Group

Other ancillary files not covered here

- **SMOKE mobile codes file (MCODES): Defines valid road class codes, vehicle type codes, and SCCs for mobile sources**
- **Biogenic land use:**
  - **County landuse (SMOKE file BCUSE)**
  - **Gridded landuse for BEIS3 (SMOKE files BELD3_A, BELD3_B, BELD3_TOT). These are netCDF I/O API files and there is not currently an easy way to create these files – we would like to add a tool to do this to SMOKE.**
- **Biogenic emission factors for summer and winter (SMOKE files BFAC and W_BFAC)**
- **Mobile information for running MOBILE6 (via SMOKE or other tools)**
- **ORIS information (assigns county and other information based on ORIS ID) – for using CEM data**
- **Meteorology data for MOBILE6 processing, plume rise, and biogenics**

Best Practices for Changing Emissions Modeling Inputs

- National files will not be all things to all people. Expect to customize to get more realistic emission inputs when looking in detail at a specific region.

- Smart to keep original and changed versions of files as you go.

- Headers and comments allow changes to be documented in file, but you must remember. Useful to include date changed, reason for the change, change description, and who.

- If needed, names of files can be changed to improve file tracking. In SMOKE, assigns files can be edited to use different file names.

Conclusion

- **Nearly all input files are ASCII files and can be changed (only exception – BEIS3 land use)**
- **File formats are available in the SMOKE documentation**
- **Lots of files to consider, so an appropriate amount of time is needed for review of the files and adapting to a specific modeling case.**
- **Hope this has been helpful!**