Emissions Modeling

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Riviera Hotel
Las Vegas, Nevada
11 April 2005
Part 1: Emissions Modeling Concepts
Emission Inventory Group

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

- **Inventory pollutant**: A compound or group of compounds defined for record-keeping and regulatory purposes (e.g. CO, NOx, VOC, PM$_{10}$)
- **Species**: 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)
- **Chemical mechanism**: A set of chemical species and their interactions used to represent air chemistry (e.g., CB-IV, RADM, SAPRC)
Definitions (2)

- **Map projection**: The mathematical representation of the spherical surface of the earth in 2-d
- **Model grid**: 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.
Spatial allocation: Convert the source spatial extent to the grid cell resolution (or census track) needed by the air quality model.

Chemical speciation: 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).

Temporal allocation: 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)

- **Profile data**: Factors used for disaggregating emissions data as is done during chemical speciation or temporal allocation.

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

- **Gridding surrogate**: 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:

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<th>15</th>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SC, All 17</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
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 × 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)

- Land use Data
- Biogenic Processing
- Mobile Processing
- Nonpoint (Area) Processing
- Point Processing
- Meteorology Data
- Emissions Inventories
- Matrices
- Hourly Layer Fractions
- Hourly Emissions
- Merge Processing
- Model-Ready Emissions
- Emissions Reports
- Optional Formatting

Emission Inventory Group
SMOKE Dataflows (2)

- Emissions Inventories
- Meteorology Data
- Profiles and X-refs
- SMOKE Inventory
- AQM Specs
- Control Data
- TEMPORAL
- Hourly Emissions
- SPCMAT
- Speciation Matrix
- GRDMAT
- Gridding Matrix
- CNTLMAT
- Control Matrix
Other Processing Paradigms

Growth and Controls -> Speciation -> Temporal Allocation -> Gridding -> Model Ready Emissions

SMOKE Processing Paradigm

Load Inventory -> Growth and Controls -> Speciation -> Temporal Allocation -> 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


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
- 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
- CAMR: ftp://airmodelingftp.com/CAMR
2001 Criteria for CAIR Overview

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

- 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
  - Livestock NH3 does not require the across-the-board 30% reduction.
  - Minor nonpoint Hg changes from 1999 NEI documented in CAMR TSD
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
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:

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<th>Profiles table</th>
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<tr>
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<td>17 0.4, 0.4, 0.2</td>
</tr>
</tbody>
</table>
Latest emissions modeling data from EPA

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/](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
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!