# Emissions Inventory Preparation for Air Quality Modeling (Base Year)

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Alison Eyth and Jeff Vukovich
EPA Office of Air Quality Planning and Standards
Emission Inventory and Analysis Group

## Goal of Class

- To introduce you to the various tasks involved with preparing emissions inputs to air quality models for base (historic) years
- To answer commonly asked questions about this process

# Course Outline and Schedule

- 8:30 Background, Inventories, Tools, and QA
- 9:00 Emissions Modeling and Plume Rise
- 9:25 Spatial Allocation
- 9:45 Temporal Allocation
- 10:15 Break
- 10:30 Fugitive Dust and Biogenic Emissions
- 10:45 Speciation
- 11:15 Onroad Mobile Sources
- 11:45 Final processing and QA steps
- 12:00 LUNCH



# Background: Purpose and Contents of a Modeling Platform

- A modeling platform provides a comprehensive air quality modeling system that uses the most recent technically sound data and state-of-the-science tools available
- Modeling platforms are used to support EPA regulations and other analyses
- Major components of a modeling platform:
  - Meteorological models (WRF) and met. data
  - Boundary conditions (GEOS-Chem)
  - **Emissions**: base year (NEI)+NonUS, future year projections
  - Air quality models (CMAQ, CAMx)
  - **Other**: ancillary data for emissions modeling, projections data, emissions modeling tools (SMOKE, etc) and scripts

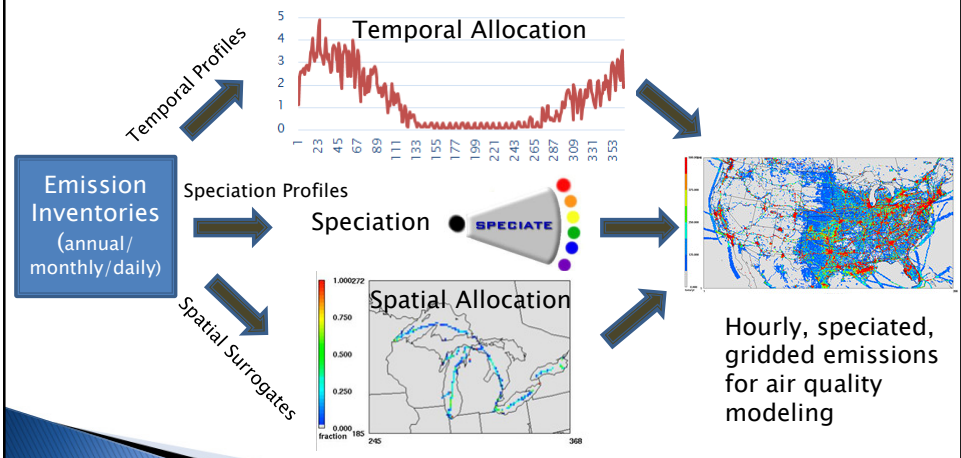
# Common Air Quality Studies

- Regulatory Impact Assessments (RIAs)
  - Model a base year focused on Criteria Air Pollutants (CAPs)
  - Model a future year base case with on-the-books rules
  - Model one or more cases that represent the rule
  - Estimate costs and benefits of rule
- National Air Toxics Assessment (NATA)
  - Model a base year including as many Hazardous Air Pollutants (HAPs) as possible
  - Compute risk based on CMAQ and AERMOD concentrations
- Transport Modeling
  - Model a base year and future year base case
  - Perform source apportionment modeling to determine contribution of states to nonattainment in other states



# Emissions Modeling Process

- Steps needed to convert emissions inventories into the resolution and formats needed by air quality models



# Performing Emissions Modeling

- We use the **Sparse Matrix Operator Kernel Emissions (SMOKE)** modeling system and associated tools to process our emissions into air quality model-ready files (http://cmascenter/smoke)
- The input **emission inventories** (e.g., NEI) can be annual, monthly, daily, or hourly
- "**Ancillary" data files** help process inventories into gridded hourly emissions of the chemical species (e.g., NO, $NO_2$, ISOP) used by the air quality model
- **Meteorological data** such as temperature, precipitation, and radiation are needed to compute emissions and for some sectors temporalization (e.g., onroad mobile, biogenic, res. wood, agricultural)
- **Quality assurance** steps and data summaries ensure data is properly transformed and mass is not lost



# Base Year Emissions from the National Emissions Inventory (NEI)

- Data is submitted by states, locals, tribes (S/L/T) and EPA into the **Emissions Inventory System (EIS)**
- Five NEI data categories
  - Point/Facility Inventory (point locations)
  - Nonpoint (county-based)
  - Onroad mobile sources
  - Nonroad mobile sources
  - Events (e.g., Fires) – day-specific point emissions
- EPA and S/L/T data are blended to create the NEI which represent emissions for a specific year
  - Full NEI produced every third year (e.g., 2011, 2014, 2017)
  - 2014 NEI version 2 coming late 2017
  - See https://www.epa.gov/air-emissions-inventories

# Recent Emission Modeling Platforms

- 2011v6.3 platform is based on 2011NEIv2
  - First number (2011) is the base year being modeled
  - The number before the "." corresponds to a specific NEI year (e.g., 6 means 2011 NEI was used)
  - The number after the "." is an iteration of the platform (e.g., 3 is a third major iteration for 2011)
  - Emission modeling platforms have both base and future years that go with them (e.g., 2017, 2023)
- 2014v7.0 is the initial 2014 NATA modeling platform based on 2014NEIv1
- A "case" is a specific set of AQM-ready emissions inputs and has an abbreviation



# EPA's Emissions Modeling Case Abbreviations – Alphabet Soup!

- Modeling case abbreviations include:
  - the **year** represented in the modeling (e.g. 2011, 2016)
  - a letter representing the NEI base year (e.g., e, f)
  - a letter representing the iteration of the emissions (e.g., a, b)
  - a year and letter representing the meteorology (e.g., 11g, 14j)
  - optionally, the speciation used (e.g., cb6cmaq, sparc07t)
  - optionally, the version of the platform (v5=2008, v6 =2011)
  - optionally, a special note about the case (e.g., nata, cntl for a control case)
- Examples
  - **2011el_cb6v2_v6_11g**: 2011= year modeled, e= 2011 NEI, l = twelfth 2011 case, cb6v2 = CB6 speciation, v6 = platform, 11g = WRF 3.5 for 2011
  - **2016fc_cb6camx_16j**: 2016 = year modeled, f = 2014 NEI, c = third case, cb6cfamx = CB6 speciation, 16j = WRF 3.8 for 2016

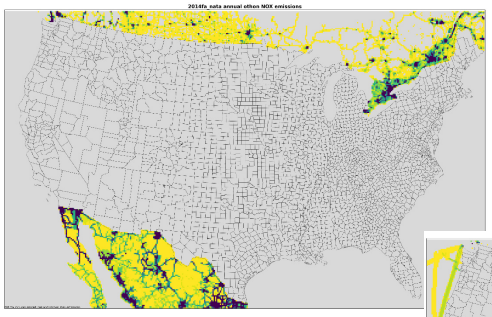
# EPA US 12km Modeling Platform Domains

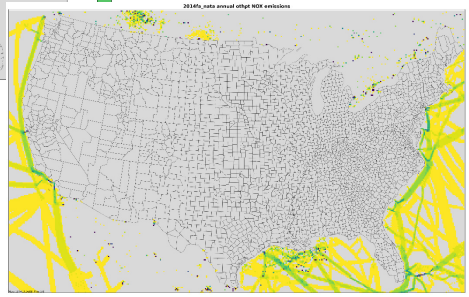
- US domains / grids use consistent map projections (Lambert)
- Other domains also exist (e.g., 36km, 4km, hemispheric)
- Many US domains include parts of Canada and/or Mexico

# Non-US emissions included in the EM platform

- Canada emissions & ancillary data (e.g., surrogates)
  - Courtesy Environment Canada
  - 2010 used until 2013 data provided in spring of 2017
  - Fire emissions provided for summer 2011 and other recent years
- Mexico 2008 emissions and projections of these
  - Based on Inventario Nacional de Emisiones de Mexico, 2008
  - MOVES-Mexico data was developed for key years
  - 2011 fire emissions for Mexico derived from **F**ire **IN**ventory from **N**CAR (**FINN**): A daily fire emissions product for atmospheric chemistry models [also used for winter in Canada]
- Biogenic emissions in Canada and Mexico are computed as part of EPA's standard processing
- Hemispheric Transport of Air Pollution (HTAP) version 2 inventories used outside of North America in the hemispheric version of the 2011 platform

# 2014fa NOx Emissions Outside of United States Boundaries





Top: Onroad sources in Canada and Mexico

Bottom: Non-US point sources and Commercial marine vessels outside of state waters



# Emissions Modeling Platform Sectors

- Emission inventories are broken down into "sectors" used to prepare AQM-ready emissions for different parts of the inventory
- Each sector has unique processing or inventory characteristics and starts with lowercase letter
- Specific sectors vary by modeling platform but cover all sources in the inventory
- Point source sectors keep their specific latitude-longitude locations throughout the process
- Nonpoint sectors are allocated to grid cells using spatial surrogates
- **EPA processes emissions separately for each sector then merges the ground-level emissions for a case together at the end**

# 2016 Platform Sectors (1 of 2)

| Point and non-US Sectors | Sector Description |
|---|---|
| ptegu | Point sources that are Electric generating units (EGUs) |
| pt_oilgas | Point sources related to oil and gas production |
| ptnonipm | Point sources that are not EGUs nor related to oil and gas |
| ptagfire | Point source day-specific agricultural fires (was agfire) |
| ptfire | Point source day-specific wild and prescribed fires |
| ptfire_mxca | Non-US point source fires |
| cmv_c3 | Category 3 (large) Commercial Marine Vessels as points |
| othpt | Non-US point sources |
| othafdust | Non-US area fugitive dust sources (Canada only) |
| othar | Non-US area (i.e., nonpoint) sources |
| onroad_can | Onroad mobile sources for Canada (was othon) |
| onroad_mex | Onroad mobile sources for Mexico (was othon) |



# 2016 Platform Sectors (2 of 2)

| Nonpoint Sectors | Sector Description |
|---|---|
| afdust_adj | Met.-adjusted area fugitive dust emissions |
| ag | Agricultural ammonia sources |
| beis | Biogenic emissions based on the BEIS model |
| cmv_c1c2 | C1&C1 Commercial marine vessels (nonpoint) |
| nonpt | Nonpoint sources not in other sectors |
| np_oilgas | Nonpoint oil and gas-production-related sources |
| nonroad | On-land mobile sources that do not drive on roads or railroads |
| onroad | On-land mobile sources that drive on roads |
| onroad_ca_adj | Onroad mobile sources in California |
| rail | Locomotive sources on railroads |
| rwc | Residential wood combustion sources |

# Building a Platform and QA

- When a new NEI version becomes available, **flat files** (a .csv format) are output from EIS and then the point and nonpoint inventories are split into sectors
  - Onroad, nonroad, and biogenic done before NEI release
  - Key inventory fields are FIPS code, pollutant, source classification code (SCC), and stack parameters
- Typically, when we build a new platform, we **compare the inventories and results** based on any new methods **to a previous platform**
  - Create difference reports by state, county, and/or SCC
  - Create charts and maps
- Update ancillary files to account for new SCCs and data
- Examples of assessments done as needed
  - Sub-annual (e.g. ozone season, hourly, daily)
  - Examine speciated PM or VOC
  - Review gridded inventory emissions



# 2014 vs 2016 Comparison

- First, prepare excel workbook by sector, state, pollutant, case 1, case 2, absolute change and percent change; then apply filters (e.g. > 1500)

| sector | state | poll | ann_emis_2014fb | ann_emis_2016fc | diff_tons | percent diff |
|---|---|---|---|---|---|---|
| ptagfire | Arkansas | PM2_5 | 1,706 | 2,745 | 1,039 | 60.90% |
| ptagfire | California | PM2_5 | 3,596 | 5,689 | 2,093 | 58.20% |
| ptagfire | Florida | PM2_5 | 3,632 | 3,676 | 44 | 1.20% |
| ptagfire | Georgia | PM2_5 | 2,090 | 1,587 | -503 | -24.10% |
| ptagfire | Kansas | PM2_5 | 10,861 | 18,385 | 7,525 | 69.30% |
| ptagfire | Missouri | PM2_5 | 1,640 | 2,368 | 728 | 44.40% |
| ptagfire | North Dakota | PM2_5 | 1,969 | 3,241 | 1,272 | 64.60% |
| ptagfire | Oklahoma | PM2_5 | 6,124 | 9,545 | 3,421 | 55.90% |
| ptagfire | Texas | PM2_5 | 4,401 | 5,815 | 1,413 | 32.10% |
| ptagfire | Washington | PM2_5 | 1,694 | 1,334 | -359 | -21.20% |

# 2014-2016 EGU comparison

| State | 2014 SO2 | 2016 SO2 | % diff SO2 | 2014 NOx | 2016 NOx | % diff NOx |
|---|---|---|---|---|---|---|
| Alabama | 119,919 | 25,337 | -79% | 50,489 | 28,674 | -43% |
| Arkansas | 76,046 | 46,706 | -39% | 38,626 | 26,968 | -30% |
| Florida | 99,628 | 40,453 | -59% | 73,740 | 62,611 | -15% |
| Illinois | 143,261 | 67,096 | -53% | 48,196 | 32,147 | -33% |
| Indiana | 294,339 | 89,911 | -69% | 110,290 | 83,170 | -25% |
| Kentucky | 201,871 | 76,290 | -62% | 86,816 | 57,586 | -34% |
| Louisiana | 76,774 | 45,851 | -40% | 46,285 | 47,462 | 3% |
| Michigan | 154,855 | 85,354 | -45% | 59,625 | 41,541 | -30% |
| Mississippi | 90,790 | 3,187 | -96% | 23,643 | 16,022 | -32% |
| Missouri | 134,326 | 100,798 | -25% | 74,883 | 57,335 | -23% |
| Ohio | 302,698 | 107,532 | -64% | 88,177 | 56,137 | -36% |
| Oklahoma | 76,791 | 49,439 | -36% | 39,450 | 25,130 | -36% |
| Pennsylvania | 278,498 | 98,839 | -65% | 129,423 | 83,300 | -36% |
| Texas | 346,244 | 247,044 | -29% | 124,892 | 108,655 | -13% |
| West Virginia | 101,586 | 42,515 | -58% | 72,631 | 52,307 | -28% |



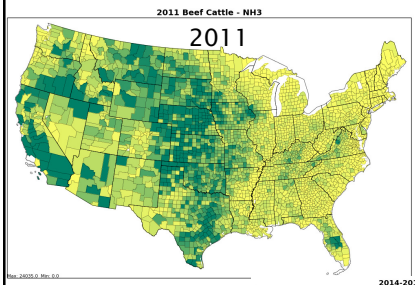
# 2014 vs 2016 County-level Comparisons

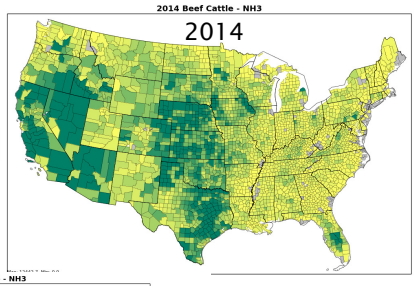
| sector | state | county | poll | ann_emis_2014fb | ann_emis_2016fc | diff | pdiff |
|---|---|---|---|---|---|---|---|
| beis | Alabama | Autauga Co | CO | 2,458 | 2,756 | 298 | 12.1% |
| beis | Alabama | Autauga Co | NOX | 157 | 167 | 10 | 6.2% |
| beis | Alabama | Autauga Co | VOC_INV | 21,332 | 23,829 | 2,496 | 11.7% |
| beis | Alabama | Baldwin Co | CO | 7,276 | 8,206 | 930 | 12.8% |
| beis | Alabama | Baldwin Co | NOX | 399 | 433 | 34 | 8.6% |
| beis | Alabama | Baldwin Co | VOC_INV | 57,200 | 63,835 | 6,635 | 11.6% |
| beis | Alabama | Barbour Co | CO | 3,417 | 3,918 | 501 | 14.7% |
| beis | Alabama | Barbour Co | NOX | 151 | 164 | 14 | 9.0% |
| beis | Alabama | Barbour Co | VOC_INV | 30,439 | 35,010 | 4,572 | 15.0% |

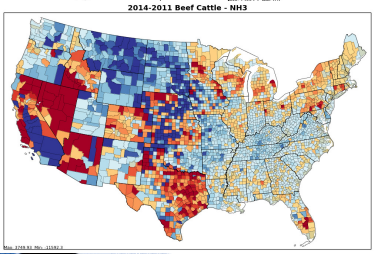
Biogenic changes mainly due to meteorology; others due to # of days in year

| sector | state | county | poll | ann_emis_2014fb | ann_emis_2016fc | diff | pdiff |
|---|---|---|---|---|---|---|---|
| ptnonipm | Alabama | Autauga Co | CO | 2,475 | 2,482 | 7 | 0.3% |
| ptnonipm | Alabama | Autauga Co | NH3 | 71 | 72 | 0 | 0.3% |
| ptnonipm | Alabama | Autauga Co | NOX | 2,530 | 2,537 | 7 | 0.3% |
| ptnonipm | Alabama | Autauga Co | PM10 | 536 | 538 | 1 | 0.3% |
| ptnonipm | Alabama | Autauga Co | PM2_5 | 428 | 429 | 1 | 0.3% |
| ptnonipm | Alabama | Autauga Co | SO2 | 3,692 | 3,702 | 10 | 0.3% |
| ptnonipm | Alabama | Autauga Co | VOC_INV | 901 | 903 | 2 | 0.3% |

# County-level Base and Difference Maps: Beef Cattle $NH_3$



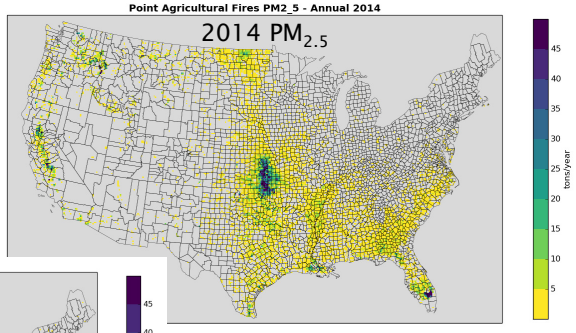

Maps help us see spatial variation and hot spots

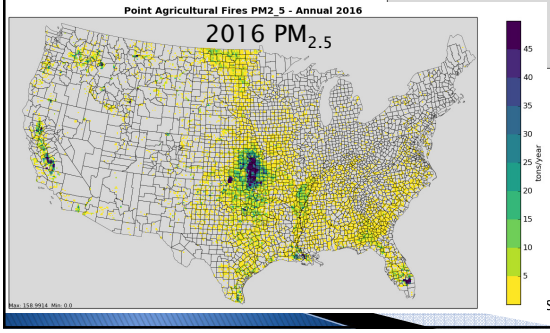
Most of our county-level maps are created with Python



# Gridded Maps: Ptagfire Example

Gridded maps can be created with VERDI, PAVE, etc.




For some sectors (e.g., fires, biogenics) we create monthly maps

# Platform Data not in the NEI

- Some modeling platform data versions are not the same as what is in the NEI
  - Corrections to issues found after the NEI release
  - New data becomes available after NEI release
  - More detailed data is available than is stored in NEI
    - Continuous Emissions Monitoring System (CEMS) data for EGUs are hourly by unit
    - Nonroad data are computed monthly (summed in the NEI)
    - Onroad and biogenics data computed as hourly emissions and then aggregated & summed for the NEI
  - NEI uses average meteorological adjustments for afdust, but the modeling platform emissions are adjusted based on hourly, gridded met. data



# Questions?

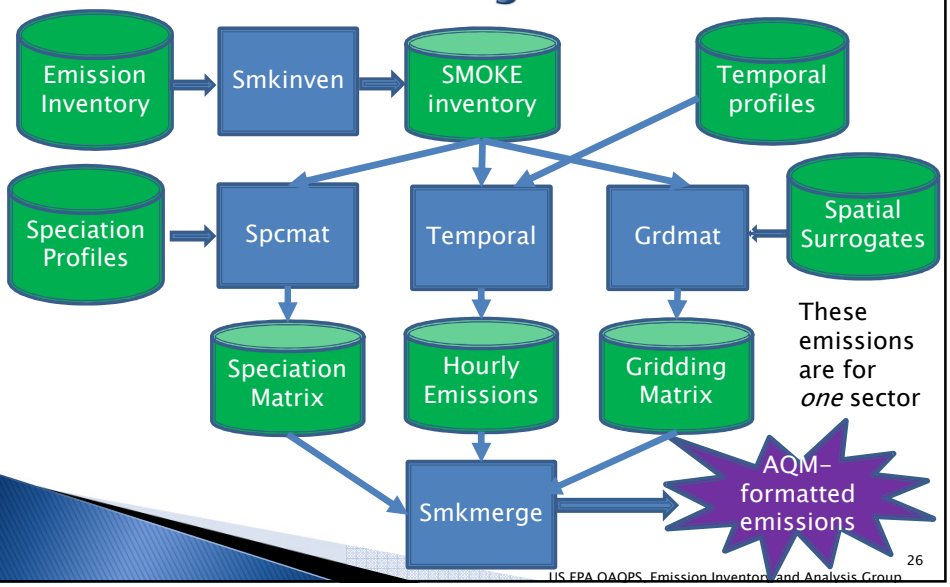
- Are there any questions on what we've covered so far?

# Emissions Modeling with SMOKE

- We use the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system and associated tools to process emissions into air quality model-ready files
  - Smkinven: reads in the emission inventories
  - Grdmat: computes gridding matrix using lat-lon locations and spatial surrogates
  - Spcmat: computes speciation matrix using speciation profiles
  - Temporal: temporally allocates emissions to hours using temporal profiles
  - Elevpoint: Splits ground-level and elevated point sources
  - Smkmerge: merges all matrices and temporalized emissions to create AQM-ready data for a sector
  - Mrggrid: merges ground-level emissions from different sectors together into a complete ground-level file



# SMOKE Data Flow for a Generic Emissions Modeling Sector




These emissions are for *one* sector

# Special Emissions Models

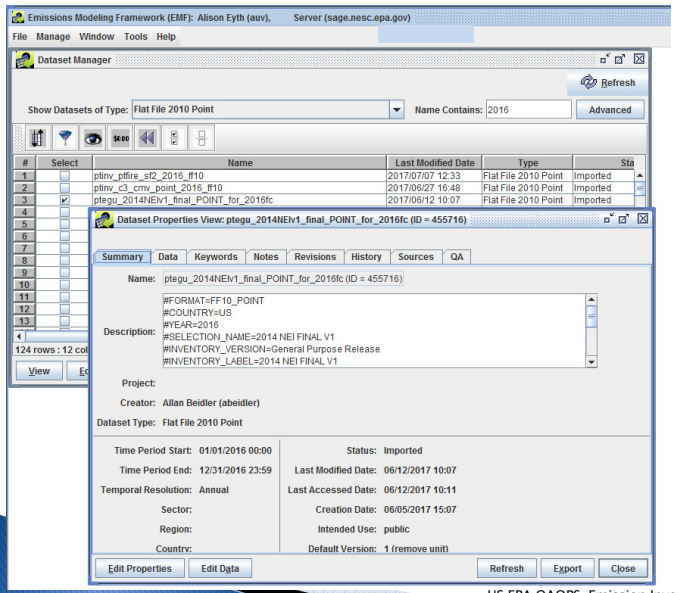
- **Biogenic Emission Inventory System (BEIS):** part of SMOKE and CMAQ that creates air quality model-ready biogenic emissions
  - SMOKE programs: Normbeis3, Tmpbeis3
- **Motor Vehicle Emission Simulator (MOVES):**
  - For *onroad* mobile sources: generates emission factors that can be combined with activity data (e.g., Vehicle miles traveled, speed) within SMOKE
    - SMOKE programs: Met4moves, Movesmrg
  - For *nonroad* mobile sources: generates county-level emission inventories for each month
    - Previously done with National Mobile Inventory Model (NMIM) and NONROAD model



# Other Emissions Modeling Tools

- Surrogate Tool: creates spatial surrogates from Shapefiles to put emissions into grid cells
- Speciation Tool: creates chemical speciation profiles from SPECIATE database profiles (e.g., NOx->NO+ $NO_2$, PM2.5->EC+OC+..., VOC->…)
- Gentpro: SMOKE program that creates meteorology-based temporal profiles
- Python: helps with QA, creates reports and maps
- Emissions Modeling Framework: graphical user interface that manages inventories and related data and modeling cases; creates summaries for QA and analysis; includes Control Strategy Tool

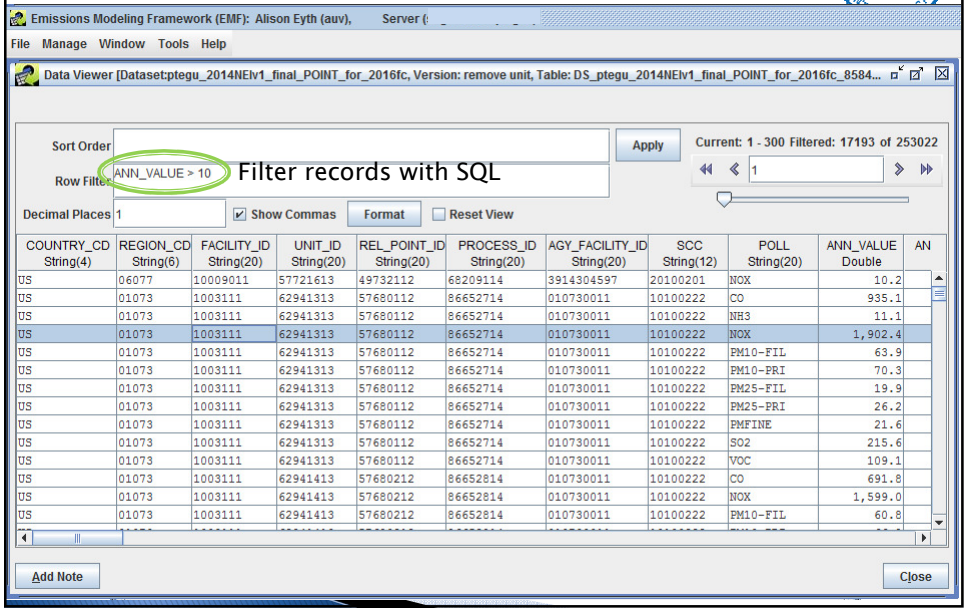
# Emissions Modeling Framework




Emission inventories are stored as Datasets in the Emissions Modeling Framework



# EMF Showing Point Inventory



# Emissions Modeling Steps for each Sector (1 of 2)

| Platform sector | Spatial | Speciation | Inventory resolution |
|---|---|---|---|
| afdust_adj | Surrogates | Yes | annual + met data |
| ag | Surrogates | Yes | annual or monthly |
| beis | Pre-gridded land use | in BEIS 3.6.1 | computed hourly |
| cmv_c1c2 | Surrogates | Yes | annual |
| nonpt | Surrogates | Yes | annual |
| nonroad | Surrogates | Yes | monthly |
| np_oilgas | Surrogates | Yes | annual |
| onroad, onroad_ca_adj | Surrogates | in MOVES 2014 | monthly activity, computed hourly |
| onroad_can | Surrogates | Yes | monthly |
| onroad_mex | Surrogates | in MOVES | monthly |
| rail | Surrogates | Yes | annual |
| rwc | Surrogates | Yes | annual |



# Emissions Modeling Steps for each Sector (2 of 2)

| Platform sector | Spatial | Speciation | Inventory resolution | Plume rise |
|---|---|---|---|---|
| othafdust | Surrogates | Yes | annual | |
| othar | Surrogates | Yes | annual | |
| othpt | Point | Yes | annual | in-line* |
| ptfire_mxca | Point | Yes | daily | In-line |
| pt_oilgas | Point | Yes | annual | in-line |
| ptegu | Point | Yes | annual & hourly CEMS | in-line |
| ptfire | Point | Yes | daily | in-line |
| ptagfire | Point | Yes | daily | Only layer 1 |
| ptnonipm | Point | Yes | annual | in-line |
| cmv_c3 | Point | Yes | Annual | In-line |

* in-line means it can be done in CMAQ

# Plume Rise

- Plume rise allows for sources to go vertically above the first layer of the air quality model (AQM has up to 35 layers)
- The SMOKE Elevpoint program selects elevated or plume-in-grid point sources using the Briggs algorithm
  - Most sources with plume height > 20m as elevated
  - Sometimes we want all sources to have plume rise
- Plume rise can be done with the SMOKE Laypoint program to compute layer fractions for each elevated point source
  - For hemispheric application, 3-D emissions are provided to the AQM



# Plume Rise Formula

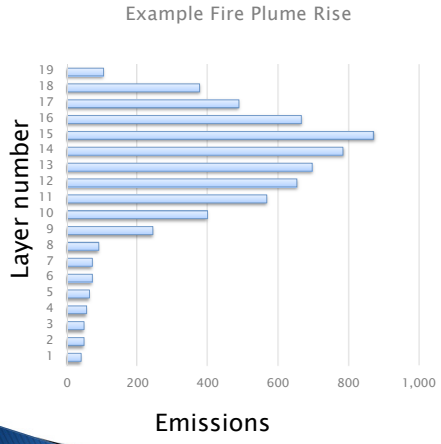
- **Stack parameters** for point sources affect plume rise
  - Height, diameter, velocity / flow, temperature
- **$F = 0.25 \times G \times V_S \times D_S^2 \times (T_S - T)/T_S$**
- For $F < 55$,
  Plume rise $= H_S + 21.313 \times F^{0.75}/U$ *otherwise*:
  Plume rise $= H_S + 38.878 \times F^{0.6}/U$ where
  - F = Bouyancy flux ($m^4/s^3$)
  - G = Mean gravitational acceleration (9.80665 $m/s^2$)
  - $V_S$ = Stack gas exit velocity (m/s)
  - $D_S$ = Inside stack diameter (m)
  - $T_S$ = Stack gas temperature (K)
  - T = Default ambient air temperature (293 K)
  - U = Default wind speed (2 m/s)
  - $H_S$ = Physical stack height (m)

# Plume Rise Requirements for AQMs Differ

- 3-D emissions files can be really big!
- CMAQ can do "in-line" plume rise
  - Provide CMAQ with 2-D hourly emissions plus locations, stack parameters, and emissions values for any elevated sources
  - Compute plume rise with hourly meteorological data
  - A special plume rise treatment is used for fires that considers acres burned and heat flux
- CAMx supports an in-line format for plume rise but does not have the same algorithm for fire plume rise
  - We run SMOKE Laypoint to compute 3-D fires
  - Point sources are then converted to CAMx format



# Allocation to Layers for AQ Modeling



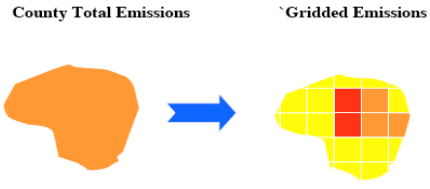
# Questions?

- Any questions on SMOKE or plume rise?
- Note: Friday presentation on new treatment for smoldering fire emissions



# Spatial Allocation

- Spatial allocation is the process of mapping inventory emissions to modeling grid cells
- There are many types of surrogates, and each has a unique code
  - Typically use SCC to X-ref surrogate to inventory
  - Population (100), Total agriculture (310), Railroad Density (261), Offshore shipping (806), Urban unrestricted AADT (222), Gas well count (698)



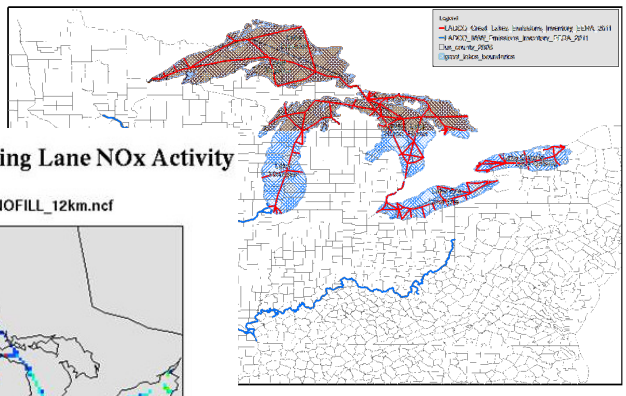
# Data Used to Create a Spatial Surrogate with Surrogate Tool

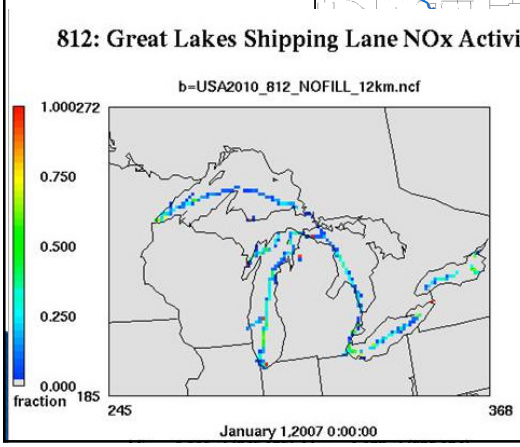
- Weight Shapefile: an attribute is selected from this spatial dataset to apportion values in a county into the model grid cells
  - Population at the census tract block level
  - Lines representing railroads
  - Point locations of oil and gas wells
- Data Shapefile: spatial dataset that represents boundaries on which inventory is computed (e.g., U.S. counties, Canadian provinces)
- Output grid or polygons: modeling grid cells, or census tracts for NATA



# Creating a CMV Surrogate

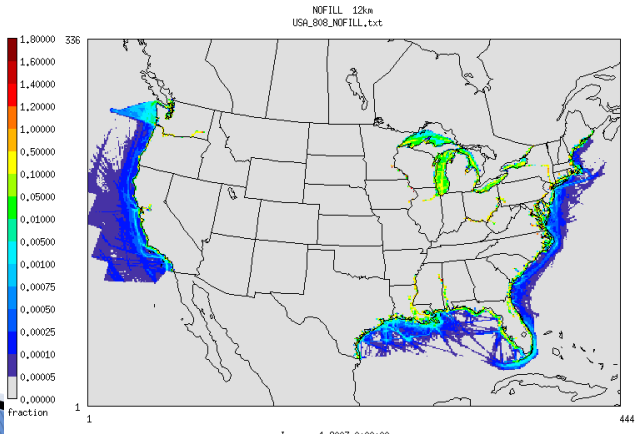
Data = US counties
Weight = NOx emissions on shipping lanes
Output is US 12km grid





# Alternative CMV Surrogate

- A new spatial surrogate based on 2013 data https://www.marinecadastre.gov/data







# Spatial Surrogate values

Value = $\frac{\text{sum of attribute in } \mathbf{grid\ cell}}{\text{sum of attribute in county}}$

*Sum to 1 for each county / province*

| Surg ID | County | Col | Row | Ratio | Comment |
|---|---|---|---|---|---|
| 806 | 01003 | 345 | 207 | 0.2 | 200/1000 |
| 806 | 01003 | 346 | 207 | 0.3 | 300/1000 |
| 806 | 01003 | 346 | 208 | 0.5 | 500/1000 |
| 806 | 01005 | 355 | 210 | 0.4 | 800/2000 |
| 806 | 01005 | 355 | 209 | 0.6 | 1200/2000 |

# Using Cross-references and Profiles (Generically)

**Cross-references and profiles are used in emissions modeling to apportion wholes into parts:**

**X-REF table**

| SCC, ID |
|---|
| 2505020121, 15 |
| 2505020122, 15 |
| 2294000000, 16 |
| 2296000000, 17 |

**Profiles table (sum to 1)**

| ID, Grid cell 1, 2, 3 | |
|---|---|
| 13 | 0.2, 0.3, 0.5 |
| 14 | 0.4, 0.4, 0.2 |
| 15 | 0.4, 0.3, 0.3 |
| 16 | 0.4, 0.5, 0.1 |
| 17 | 0.4, 0.4, 0.2 |



# Spatial Surrogate Cross reference

| FIPS ST/CTY* | SCC** | Surrogate ID | Comments |
|---|---|---|---|
| 000000 | 0040600241 | 801 | ! All counties |
| 000000 | 0040600242 | 801 | ! All counties |
| 000000 | 2505020121 | 801 | ! All counties |
| 048243 | 20100102 | 693 | ! Replaced 698 |
| 048243 | 20200201 | 693 | ! Replaced 698 |
| 008001 | 20100102 | 689 | |

*A surrogate can be applied to all counties using code 000000 or to specific states with 037000 or to specific counties

** Specific SCC assignments are always used (no hierarchy)

# Some Spatial Surrogate Data Sources

- 2011 National Land Cover Database (NLCD)
- U.S. Census American Community Survey
- U.S. Census **T**opologically **I**ntegrated **G**eographic **E**ncoding and **R**eferencing (TIGER) data
- U.S. DOT Highway Performance Monitoring System (HPMS) – Annual Average Daily Travel
- National Transportation Atlas Database
- 2014 NEI Oil and Gas Activity Data
- 2014 NEI Ports and Shipping Lanes



# Key Spatial Surrogates for CAPs

| Sector | ID | Description | NH3 | NOX | PM2_5 | VOC |
|---|---|---|---|---|---|---|
| ag | 310 | NLCD Total Agriculture | 3,135,285 | | | |
| onroad | 307 | NLCD All Development | | 560,112 | 12,560 | 1,142,592 |
| onroad | 222 | Urban Unrestricted AADT | 42,001 | 1,223,593 | 54,345 | 376,209 |
| nonpt | 306 | NLCD Med + High | 22,268 | 239,863 | 290,187 | 864,662 |
| onroad | 232 | Rural Unrestricted AADT | 25,027 | 987,683 | 33,882 | 201,764 |
| nonpt | 100 | Population | 32,222 | 0 | 0 | 1,137,409 |
| afdust | 310 | NLCD Total Agriculture | | | 1,169,400 | |
| afdust | 304 | NLCD Open + Low | | | 1,116,883 | |
| np_oilgas | 694 | Oil Production at Oil Wells | 0 | 4,375 | 0 | 1,104,120 |
| np_oilgas | 698 | Well Count – Gas Wells | 15 | 388,677 | 6,726 | 623,925 |
| onroad | 202 | Urban Restricted AADT | 24,687 | 790,075 | 30,439 | 149,645 |
| rail | 271 | NTAD Class 1 2 3 Railroad Density | 362 | 767,307 | 22,868 | 39,121 |

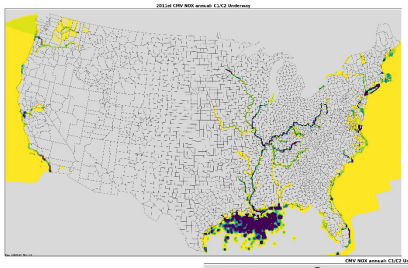
# Quality Assurance of Spatial Allocation

- Check SMOKE logs to ensure all sources have reference to spatial allocation profiles and only emissions outside the domain are not allocated.
- Review gridded emission plots by sector to ensure spatial patterns are reasonable (US sources are all in US, onshore emissions are all on land)
- Check inventory coordinate locations within counties compared to inventory FIPS.
- Compare post-SMOKE emissions to the inventory also helps to ensure that no emissions are dropped due to gridding.

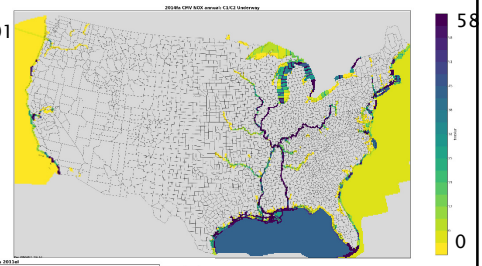


# Maps Help us to Check Spatial Surrogates: cmv_c1c2 Example

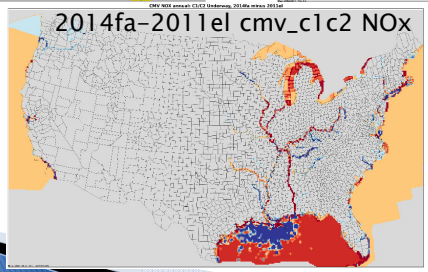
2011el cmv_c1c2 NOx




2014fa cmv_c1c2 NOx




2014fa-2011el cmv_c1c2 NOx



# Surrogate Tool

- Java program that takes .csv files as input
- Runs the Spatial Allocator to prepare surrogates
- Both are distributed by cmascenter.org
- Performs gapfilling of surrogates
  - When attributes used to compute a surrogates do not exist for a county, another surrogate is used
- Outputs quality assurance products
  - Sum of surrogate for each county (=1.0?), gapfilling
- Some datasets are too large to process with the Spatial Allocator
  - Working on using PostgreSQL with PostGIS to process these



# Questions?

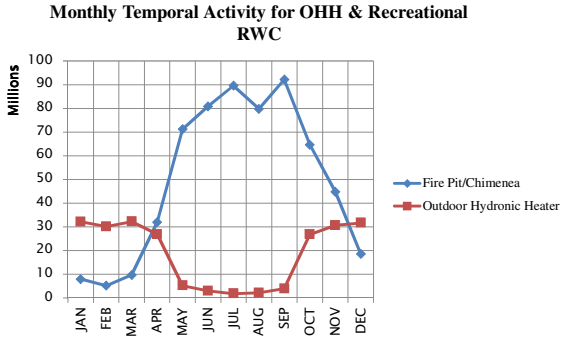
- In this section we've covered some details on spatial allocation

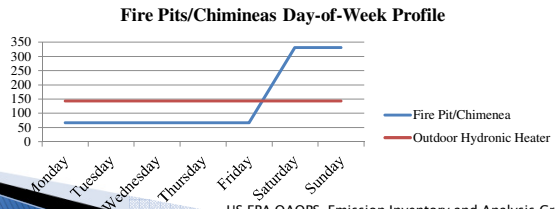
# Temporal Allocation

- Temporal allocation is the process of allocating inventory emissions to hourly emissions
- Hierarchy of temporal allocation steps: annual -> month -> day -> hour
- There are many types of temporal profiles for each resolution and each has a unique code
  - Typically, SCCs are used to map temporal profiles to inventory sources
  - Cross reference may also use FIPS, pollutant, etc.
- More control with the format in SMOKE 3.6+
  - e.g., Monday diurnal profile vs Friday diurnal profile
  - Database-friendly for use in EMF

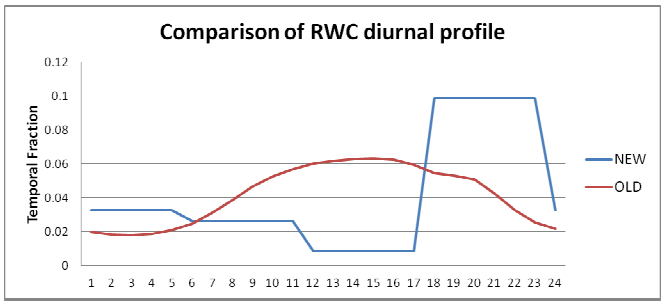


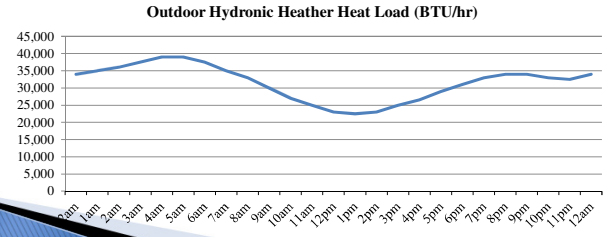
# Temporal Profile Examples (1/2)



# Temporal Profile Examples (2/2)






# Excerpt from Temporal Cross Reference and Profile Files

| SCC | FIPS | Facility | Unit | Releasept | process | Pollutant | Profile Type | Profile Num | Comment |
|---|---|---|---|---|---|---|---|---|---|
| 2104009000 | 56045 | | | | | 0 | MONTHLY | 17001 | |
| 2104009000 | 56045 | | | | | 0 | DAILY | 56045 | |
| 2104009000 | 56045 | | | | | 0 | ALLDAY | 600 | |
| 2104008700 | | | | | | 0 | MONTHLY | 17750 | "Fire pit" |
| 2104008700 | | | | | | 0 | WEEKLY | 61500 | "Fire pit" |
| 2104008700 | | | | | | 0 | ALLDAY | 600 | "Fire pit" |
| 2104008610 | | | | | | 0 | MONTHLY | 17751 | "Hydronic heater" |
| 2104008610 | | | | | | 0 | WEEKLY | 7 | "Hydronic heater" |
| 2104008610 | | | | | | 0 | ALLDAY | 1500 | "hydronic heater" |

| MonthID | Jan | Feb | Mar | Apr | May | June | July | Aug | Sept | Oct | Nov | Dec |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 17750 | 0.01 | 0.01 | 0.02 | 0.05 | 0.12 | 0.14 | 0.15 | 0.13 | 0.15 | 0.11 | 0.08 | 0.03 |
| 17751 | 0.14 | 0.13 | 0.14 | 0.12 | 0.02 | 0.01 | 0.01 | 0.01 | 0.02 | 0.12 | 0.13 | 0.15 |

| WeekID | Sun | Mon | Tue | Wed | Thu | Fri | Sat | |
|---|---|---|---|---|---|---|---|---|
| 7 | 0.14 | 0.14 | 0.14 | 0.14 | 0.14 | 0.14 | 0.14 | Equal days |
| 61500 | 0.07 | 0.07 | 0.07 | 0.07 | 0.07 | 0.33 | 0.33 | Fire pit/chimenea |

| HourID | hr0 | hr1 | hr2 | hr3 | hr4 | hr5 | hr6 | hr7 | hr8 | hr9 | hr10 | hr11 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 600 | 0.03 | 0.03 | 0.03 | 0.03 | 0.03 | 0.03 | 0.03 | 0.03 | 0.03 | 0.03 | 0.03 | 0.01 |
| 1500 | 0.04 | 0.05 | 0.05 | 0.05 | 0.05 | 0.05 | 0.05 | 0.05 | 0.04 | 0.04 | 0.04 | 0.03 |

# Temporal Settings by Sector

| Platform sector short name | Inventory resolutions | Monthly profiles used? | Daily temporal approach | Merge processing approach | Process Holidays as separate days |
|---|---|---|---|---|---|
| afdust_adj | Annual | Yes | week | all | Yes |
| ag | Annual and Daily | Yes | all, hourly met | all | Yes |
| agfire | Annual | Yes | mwdss | mwdss | Yes |
| ptagfire | Daily | No | all | all | Yes |
| beis | Hourly | No | n/a | all | Yes |
| cmv | Annual | Yes | aveday | aveday | No |
| rail | Annual | Yes | aveday | aveday | No |
| nonpt | Annual | Yes | week | week | Yes |
| nonroad | Monthly | No | mwdss | mwdss | Yes |
| np_oilgas | Annual | Yes | week | week | Yes |
| onroad | Annual & monthly[1] | No | all | all | Yes |
| onroad_ca_adj | Annual & monthly[1] | No | all | all | Yes |
| othafdust_adj | Annual | Yes | week | all | No |
| othar | Annual & monthly | Yes | week | week | No |
| onroad_can & mex | Monthly | No | week | week | No |
| othpt | Annual | Yes | mwdss | mwdss | No |
| pt_oilgas | Annual | Yes | mwdss | mwdss | Yes |
| ptegu | Daily & hourly | No | all | all | Yes |
| ptnonipm | Annual | Yes | mwdss | mwdss | Yes |
| ptfire and ptfire_mxca | Daily | No | all | all | Yes |
| rwc | Annual | No | met-based | all | Yes |

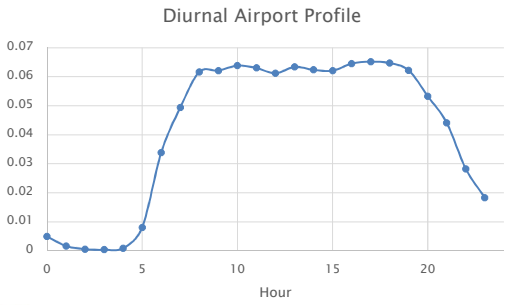


# Temporal Profile Data Sources

- Some temporal profiles have been around a while
- We look for data sources that can be used for updating temporal profiles
- Sometimes temporal profile updates happen as a result of reviewing model performance issues
  - Recently EGU profiles for municipal waste combustors and nonroad profiles for construction and lawn and garden sources have been adjusted
- To update profiles, we use studies or data when possible (e.g., rwc), otherwise we try to apply common sense knowledge of the source sector

# Airport Temporalization (1/2)

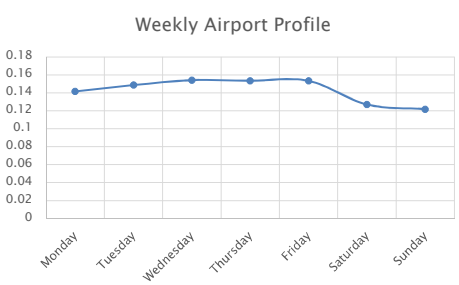
- Airport diurnal temporal profiles updated for 2014v7.0 platform based on Aviation System Performance Metrics (ASPM) Airport Analysis
  - https://aspm.faa.gov/apm/sys/AnalysisAP.asp

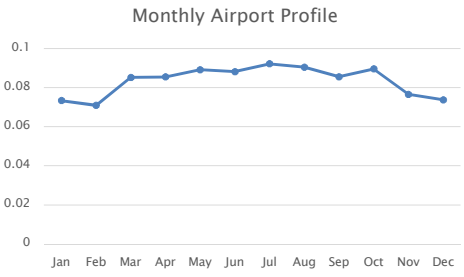





# Airport Temporalization (2/2)

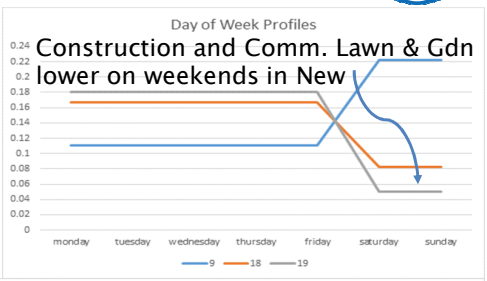
- Weekly and monthly profiles based on FAA Operations Network Air Traffic Activity System
  - http://aspm.faa.gov/opsnet/sys/Terminal.asp

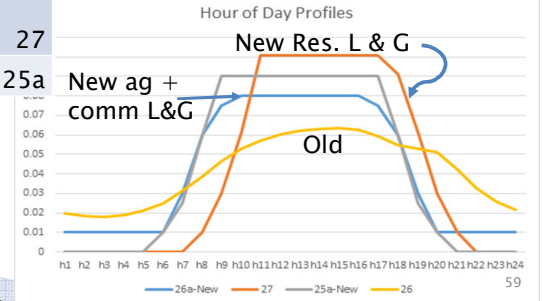


# Nonroad Temporal Profile Updates

| Non-Road Category | Old Day of Week | New Day of Week | Old Hour of day | New Hour of Day |
|---|---|---|---|---|
| Construction | 18 | 19 | 26 | 26a |
| Commercial Lawn and Garden | 18 | 19 | 26 | 25a |
| Residential Lawn and Garden | 9 | 9 | 26 | 27 |
| Agriculture | 18 | 18 | 26 | 25a |




New diurnal profiles have lower overnight emissions

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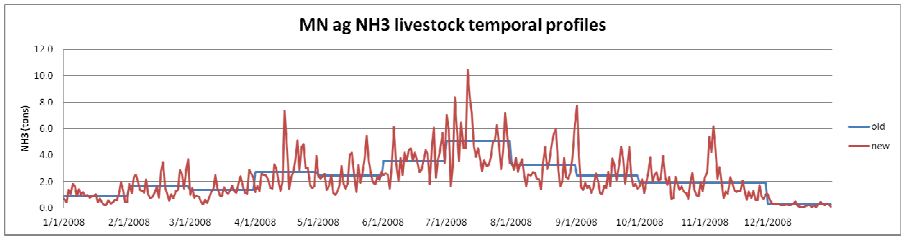
# Meteorology-based Temporalization

- Some sectors have a significant temporal variation based on changes in the meteorology
- GenTPRO
  - SMOKE program that reads gridded meteorology and spatial surrogates
  - Produces county-specific meteorology based profiles
  - Platform sectors: ag and rwc
- Other sectors influenced by meteorology
  - Area fugitive dust (afdust)
  - Biogenic emissions
  - Onroad (discussed later)
  - EGUs (indirectly)

# GenTpro: ag livestock

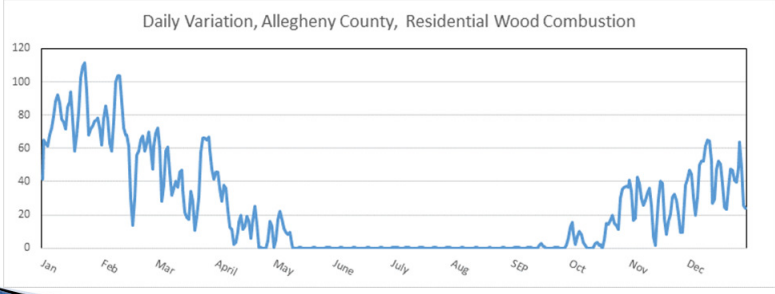
- Meteorological fields used: temperature, wind speed, and aerodynamic resistance
- Allocate monthly emissions to hour of month






# Residential Wood Day-specific Temporal Allocation with GenTpro

- Daily minimum temperature used to help allocate annual emissions to days of year
- If min temp. above 50 degrees, no emissions
  - Southern states use 60 degrees threshold

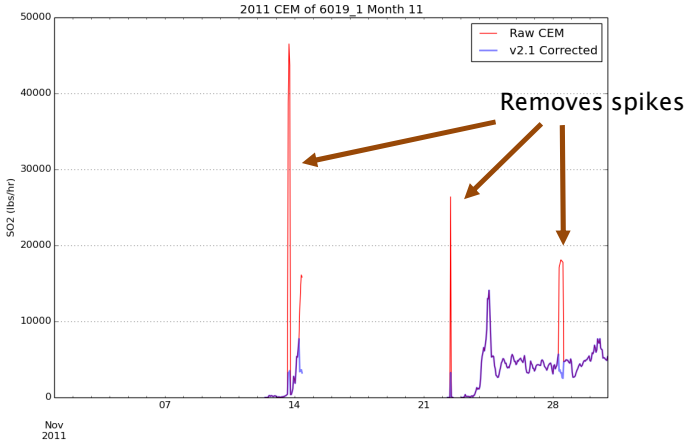


# Special Steps for EGUs

1. Separate EGUs from nonEGUs in EIS flat file based on whether IPM_YN column is non-blank
2. Download latest CEMS data for base year of interest
3. Review the assignments to ORIS IDs in the flat file and how they match up to the CEMS data
4. Identify partial year CEMS reporters
5. Run cemcorrect program to remove non-measured anomalies
6. Generate region/fuel-specific average temporal profiles for temporalization of sources without CEMS
7. Generate region/fuel-specific seasonal hourly profiles
8. Generate pseudo-hourly CEMs for partial year reporters using region/fuel temporal profiles



# Outputs from UNC's CEMS Data Correction Tool



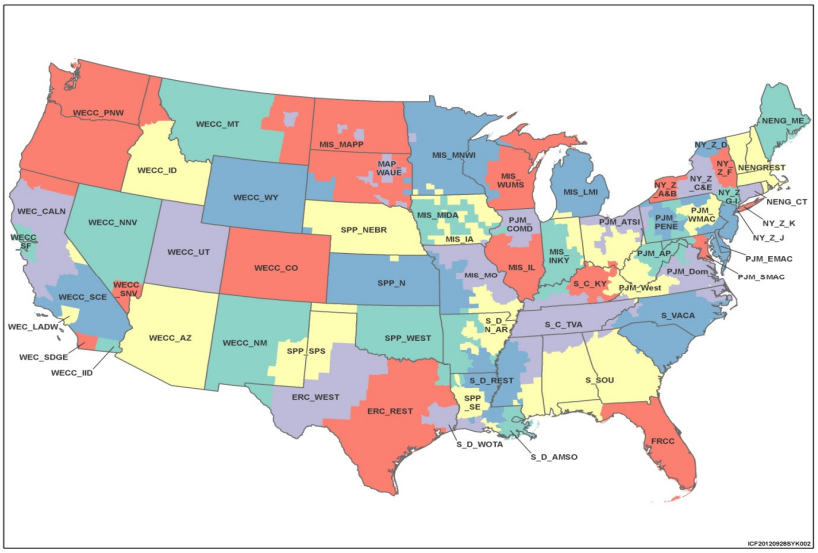

Emissions spikes adjusted to average values when they are not flagged as measured in CEMS data flags

# EGU Temporal Profiles and Matching

- Removed non-measured data values from CEMS data to ignore emission spikes
- Hierarchy of CEMS assignments:
  1. Use CEMS for all months (units with complete CEMS data) <-- **Note: CEMS data replace the annual NEI data**
  2. Use CEMS for months where have measurements, use regional averages for period without measurements (partial-year reporters)
  3. Use regional averages (units without CEMS)
- Regional average profiles
  - IPM region- and fuel-specific average profiles used
  - Different winter and summer versions of hourly profiles
- Matching of CEMS database units and IPM units with EIS/platform point sources is key

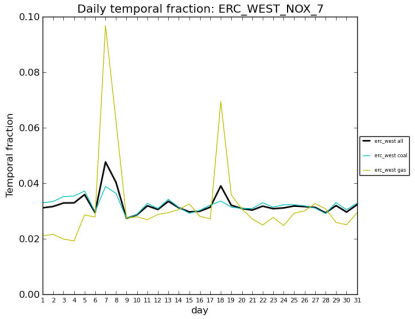


# Map of IPM regions

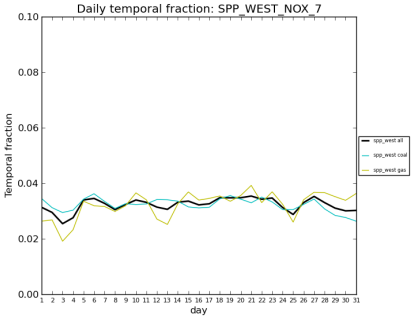


# Average Month-day Profiles: Region- and fuel-specific

Profiles differ between regions
(yellow=gas, blue=coal, black=composite)



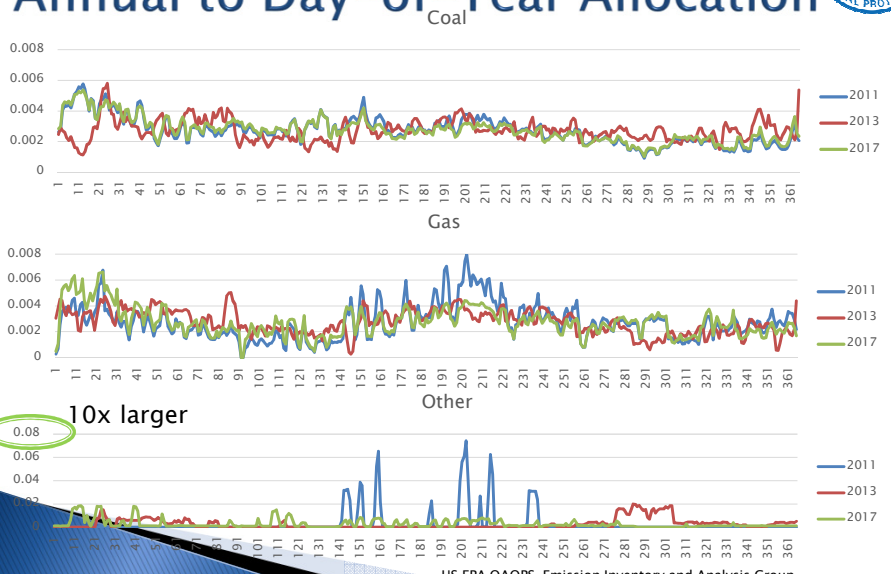

IPM Region in W Texas



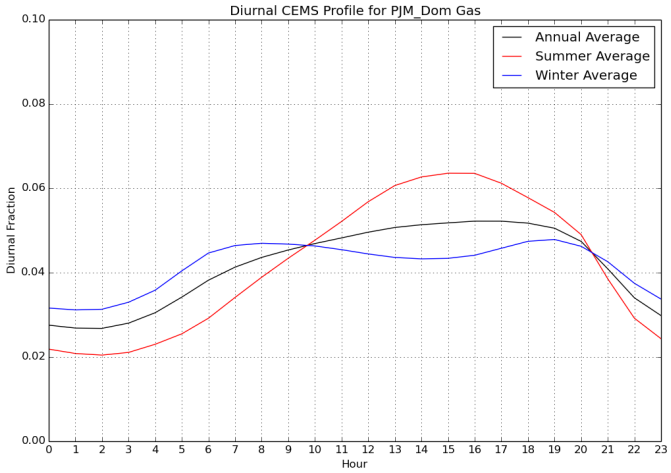

IPM Region in E Oklahoma and W Arkansas



# Mid-Atlantic CEMS Examples of Annual to Day-of-Year Allocation



# Average Profiles: Winter vs. Summer




IPM region- and fuel-specific profile – mid-Atlantic



# QA of Temporal Allocation

- Check SMOKE temporal logs to ensure all sources have reference to temporal profiles
- Sum post-SMOKE daily emissions by sector to compare back to annual for inventory comparison
- Perform various specialized analysis of EGUs (partial year reporters, spikes in CEMs data)
- Check the PTSUP files to confirm that sources are using the correct temporal profiles (i.e. that SMOKE is applying the xref correctly)
- Compare daily Smkmerge reports for rwc and ag for two different Tuesdays (for example) in the same month; those should be different (except NH3_FERT) due to the Gentpro temporalization

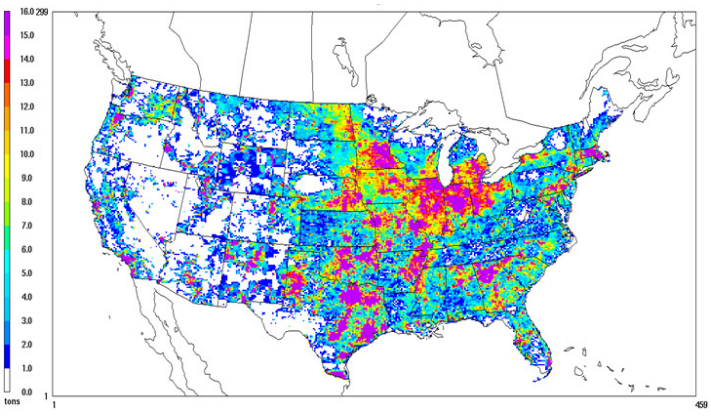
# Questions?

- Does anyone have questions on temporal allocation?



# Unadjusted Fugitive Dust

- In NEI and Platform, dust emissions are adjusted



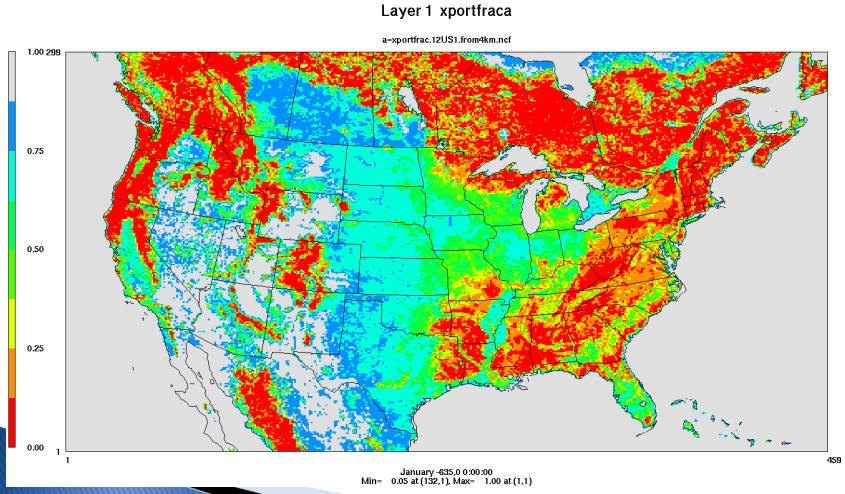
# Afdust Adjustments: Transport Fraction

- AQ models tend to overestimate the impact of fugitive dust emissions
- Prior to modeling, fugitive dust emissions are reduced according to a gridded transport fraction
- Transport fraction reduction factors depend on land use
  - Forested areas will have a lower transport fraction (higher reduction)
  - Wide open areas will have a higher transport fraction (lower reduction)
- Additional meteorologically-based reductions for rain and snow-cover are applied to fugitive dust emissions later in the process



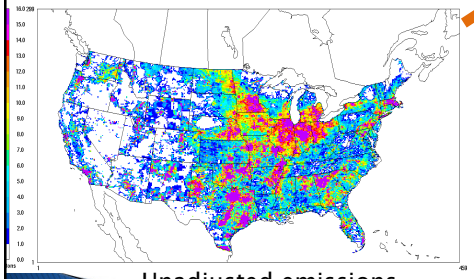
# Transport Fraction Plot

Red = high level of reduction; Gray = little reduction



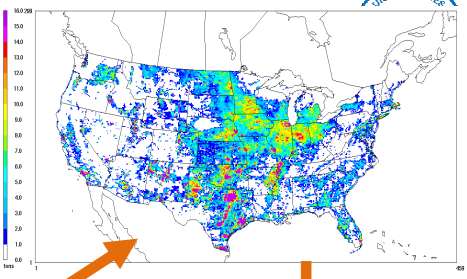
# Impact of afdust Adjustments

- Transport fraction
- Precipitation adjustment
  - Zero out hourly emissions when rain (> 0.01 inches) or there is snow)

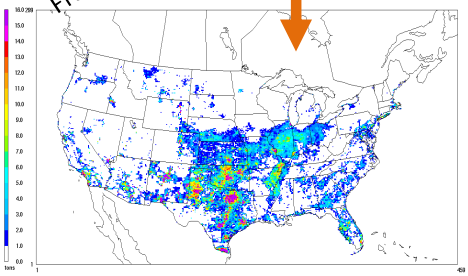


Unadjusted emissions

Apply Transport Fraction



Precipitation adjustment





# BEIS 3.6.1: Updated Biogenic Emissions

- Updated leaf temperature algorithm
  - Leaf temperature calculated using canopy model rather than 2 meter temperature
- BELD 4.1 land use based on:
  - U.S. National Land Cover Database (NLCD) 2011
  - Moderate Resolution Imaging Spectroradiometer (MODIS) for Canada and Mexico
  - Forest areas constrained by canopy coverage
  - 2011 USDA Cropland Data Layer
- Tree species from USFS Forest Inventory and Analysis (FIA) data
  - Selected surveys from 2001 to 2014 to get a complete decadal US survey that bounds the years being modeled
- SMOKE programs used:
  - Normbeis3: normalized biogenic emissions
  - Tmpbeis3: outputs gridded, ***speciated***, hourly emissions

# Meteorological Variables Needed for BEIS 3.61

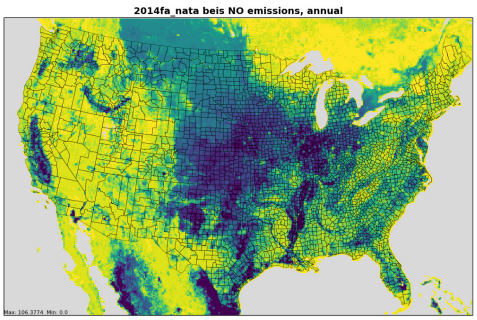
| Variable | Description |
|---|---|
| LAI | leaf-area index |
| PRSFC | surface pressure |
| Q2 | mixing ratio at 2 m |
| RC | convective precipitation per met TSTEP |
| RGRND | solar rad reaching sfc |
| RN | nonconvective precipitation per met TSTEP |
| RSTOMI | inverse of bulk stomatal resistance |
| SLYTP | soil texture type by USDA category |
| SOIM1 | volumetric soil moisture in top cm |
| SOIT1 | soil temperature in top cm |
| TEMPG | skin temperature at ground |
| USTAR | cell averaged friction velocity |
| RADYNI | inverse of aerodynamic resistance |
| TEMP2 | temperature at 2 m |



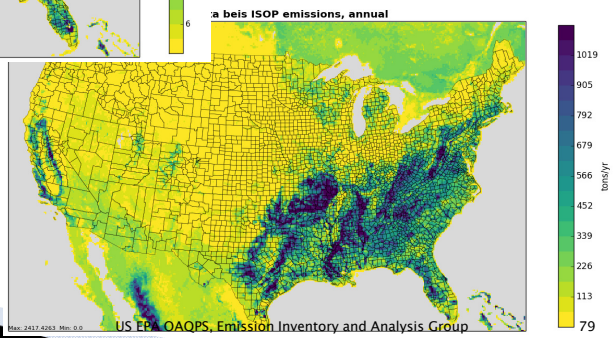
# Species Produced by BEIS

- Carbon Monoxide (CO), Nitrogen Oxide (NO)
- Acetaldehyde (ALD2),
- Higher acetaldehyde (ALDX)
- Formaldehyde (FORM)
- Isoprene (ISOP)
- Terpene (TERP)
- Sesquiterpene (SESQ)
- Ethene (ETH), Ethane (ETHA)
- Internal (IOLE) and terminal olefins (OLE)
- Ethanol (ETOH), Methanol (MEOH)
- Paraffins (PAR)
- No PM species…

# 2014 Annual Biogenic Emissions




- Top: NO from soil (depends on temperature, precipitation, and fertilizer)




- Bottom: Isoprene (produced during photosynthesis)



# Questions?

- Any questions on fugitive dust or biogenic emissions?

# Speciation

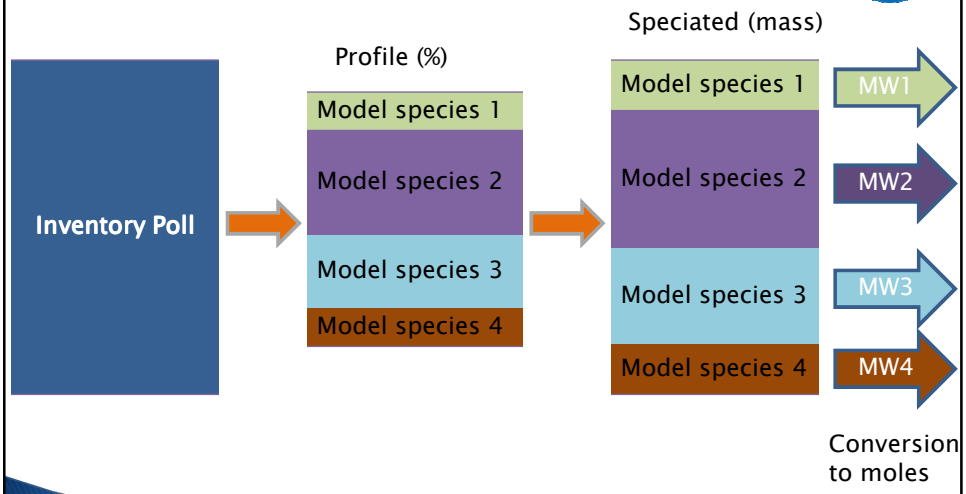
- Mapping inventory pollutants to model species
  - Model species are used in the AQM
  - NOx, VOC (TOG), and PM are speciated
- There are many types of speciation profiles and each has a unique code
  - Typically use SCC **and** pollutant to X-ref speciation profile to inventory source
  - Cross reference may also use FIPS, facility, etc.
- Different chemical mechanisms:
  - Emissions should match chemical mechanism of AQM
  - Different mechanisms have different list of model species
  - Examples: CB05, CB6, SAPRC07



# Obtaining Speciation Profiles

- SPECIATE database
  - Source of most speciation profiles in the platform
  - SPECIATE 4.5 is the most recent version
  - Includes basin-specific profiles for oil and gas sources
  - https://www.epa.gov/air-emissions-modeling/speciate-version-45-through-40
- Speciation Tool
  - Processes profiles from the SPECIATE database into the chemical mechanisms used by air quality models
  - Written in PostgreSQL and Perl
  - Separate training class for Speciation Tool
  - Available from cmascenter.org

# Speciation Overview






# NOx Speciation

- NOx is converted to following model species:
  - NO
  - NO2
  - HONO
- Example profiles:

| profile | pollutant | species | massfrac |
|---|---|---|---|
| HONO | NOX | NO2 | 0.092 |
| HONO | NOX | NO | 0.900 |
| HONO | NOX | HONO | 0.008 |
| NHONO | NOX | NO2 | 0.100 |
| NHONO | NOX | NO | 0.900 |

# $PM_{2.5}$ Speciation

- Older versions of CMAQ had "simplified" PM model species (AE5)
- Recent versions of CMAQ have the aerosol module ISORROPIA v2 that requires additional PM model species (AE6)

| species name | species description | AE5 | AE6 |
|---|---|---|---|
| POC | organic carbon | Y | Y |
| PEC | elemental carbon | Y | Y |
| PSO4 | sulfate | Y | Y |
| PNO3 | nitrate | Y | Y |
| PMFINE | unspeciated PM2.5 | Y | N |
| PNH4 | ammonium | N | Y |
| PNCOM | non-carbon organic matter | N | Y |
| PFE | iron | N | Y |
| PAL | aluminum | N | Y |
| PSI | silica | N | Y |
| PTI | titanium | N | Y |
| PCA | calcium | N | Y |
| PMG | magnesium | N | Y |
| PK | potassium | N | Y |
| PMN | manganese | N | Y |
| PNA | sodium | N | Y |
| PCL | chloride | N | Y |
| PH2O | water | N | Y |
| PMOTHR | unspeciated PM2.5 | N | Y |

Prescribed Burning Composite Prof. (91109)

| pollutant | species | massfrac |
|---|---|---|
| PM2_5 | POC | 0.5019 |
| PM2_5 | PEC | 0.1093 |
| PM2_5 | PSO4 | 0.0033 |
| PM2_5 | PNO3 | 0.0107 |
| PM2_5 | PNH4 | 0.0034 |
| PM2_5 | PAL | 0.0005 |
| PM2_5 | PCA | 0.0007 |
| PM2_5 | PCL | 0.0024 |
| PM2_5 | PFE | 0.0004 |
| PM2_5 | PK | 0.0014 |
| PM2_5 | PMN | 0.0001 |
| PM2_5 | PMOTHR | 0.0125 |
| PM2_5 | PNA | 0.0014 |
| PM2_5 | PNCOM | 0.3513 |
| PM2_5 | PSI | 0.0001 |
| PM2_5 | PTI | 0.0007 |



# VOC Speciation

- Inventory VOC is converted to Total Organic Gas (TOG)
  - Example for Gas Exh E10: VOC * 1.199 = TOG
- TOG is then speciated according to the mechanism (species sum to 1.0):
  - Different model species depending on the chemical mechanism (e.g., CB05)

| Model Species | Description |
|---|---|
| ALD2 | Acetaldehyde |
| ALDX | Propionaldehyde and higher aldehydes |
| BENZENE | Benzene* |
| CH4 | Methane* |
| ETH | Ethene |
| ETHA | Ethane |
| ETOH | Ethanol |
| FORM | Formaldehyde |
| IOLE | Internal olefin carbon bond |
| ISOP | Isoprene |
| MEOH | Methanol |
| OLE | Terminal olefin carbon bond |
| PAR | Paraffin carbon bond |
| TOL | Toluene and other monoalkyl aromatics |
| XYL | Xylene and other polyalkyl aromatics |

Gasoline Exhaust – E10 (8751a)

| pollutant | species | massfrac |
|---|---|---|
| TOG | ALD2 | 0.0145 |
| TOG | ALDX | 0.0023 |
| TOG | CH4 | 0.1416 |
| TOG | ETH | 0.0596 |
| TOG | ETHA | 0.0234 |
| TOG | ETOH | 0.0157 |
| TOG | FORM | 0.0145 |
| TOG | IOLE | 0.0130 |
| TOG | OLE | 0.0457 |
| TOG | PAR | 0.3860 |
| TOG | TOL | 0.1044 |
| TOG | UNR | 0.0563 |
| TOG | XYL | 0.1229 |

# VOC Integration (1 of 3)

- Integration
  - Process of taking select VOC HAPs from the inventory as "true" and then speciating the remaining VOC
  - Want to avoid double counting
  - Want to speciate the remaining VOC taking into account HAPs that were removed
- BAFM
  - Benzene, Acetaldehyde, Formaldehyde, Methanol
  - List of explicit VOC HAPs
- NONHAPTOG
  - Remaining TOG after removing explicit VOC HAPs
  - NONHAPVTOG = TOG – Total of BAFM species



# VOC Integration (2 of 3)

Gasoline Exhaust – E10 (8751a)

No integrate

| pollutant | species | massfrac |
|---|---|---|
| TOG | ALD2 | 0.0145 |
| TOG | ALDX | 0.0023 |
| TOG | CH4 | 0.1416 |
| TOG | ETH | 0.0596 |
| TOG | ETHA | 0.0234 |
| TOG | ETOH | 0.0157 |
| TOG | FORM | 0.0145 |
| TOG | IOLE | 0.0130 |
| TOG | OLE | 0.0457 |
| TOG | PAR | 0.3860 |
| TOG | TOL | 0.1044 |
| TOG | UNR | 0.0563 |
| TOG | XYL | 0.1229 |

Integrate

| pollutant | species | massfrac |
|---|---|---|
| NONHAPTOG | ALD2 | 0.0019 |
| NONHAPTOG | ALDX | 0.0025 |
| NONHAPTOG | CH4 | 0.1519 |
| NONHAPTOG | ETH | 0.0639 |
| NONHAPTOG | ETHA | 0.0251 |
| NONHAPTOG | ETOH | 0.0169 |
| NONHAPTOG | FORM | 0.0010 |
| NONHAPTOG | IOLE | 0.0139 |
| NONHAPTOG | OLE | 0.0491 |
| NONHAPTOG | PAR | 0.4067 |
| NONHAPTOG | TOL | 0.1119 |
| NONHAPTOG | UNR | 0.0234 |
| NONHAPTOG | XYL | 0.1318 |

# VOC Integration (3 of 3)

| Platform Sector | Approach for integrating |
|---|---|
| ptegu | No integration |
| ptnonipm | No integration |
| ptfire, ptagfire | No integration |
| othfire | No integration |
| othar | No integration |
| othpt | No integration |
| onroad_can | No integration |
| onroad_mex | Full integration (MOVES-Mexico) |
| ag | N/A – sector contains no VOC |
| afdust, othafdust | N/A – sector contains no VOC |
| beis | N/A – contains specific VOC model species |
| nonpt, rail | Partial integration (BAFM; EBAFM for future year PFC) |
| np_oilgas | Partial integration (BAFM) |
| pt_oilgas | Partial integration (BAFM) |
| rwc | Partial integration (BAFM) |
| nonroad | Full integration (BAFM) |
| cmv_c1c2 | Full integration (BAFM) |
| cmv_c3 | Full integration (BAFM) |
| onroad | Full integration (calculated in the MOVES2014 model)* |



# Additional Speciation Concepts

- NBAFM = integration of BAFM + naphthalene
  - CMAQ CB6 has naphthalene as explicit species
  - Used for 2014-16 platforms
- COMBO files
  - Method of combining 2 or more speciation profiles by pollutant/geography
  - Example: combine E0 and E10 fuel profiles for portable fuel containers
- Speciation can be used to group/track interrelated pollutants e.g., PAH's for NATA

# Onroad speciaton

- MOVES2014a does most of the needed speciation
  - Has different profiles for different vehicle model years, regulatory classes, fuel types, and emission processes
  - Previously used COMBO files or weighted profiles to approximate, but it was a coarse approach
  - Can do an explicit mapping of profiles to sources if doing speciation within MOVES
- PM2.5
  - AE6 species coming directly from MOVES (in mass)
- VOC
  - 16 pollutants are explicit, i.e. integrated
  - Model species (moles) and inventory pollutants (mass) come directly from MOVES
  - Need to specify chemical mechanism in the MOVES run



# QA of Speciation

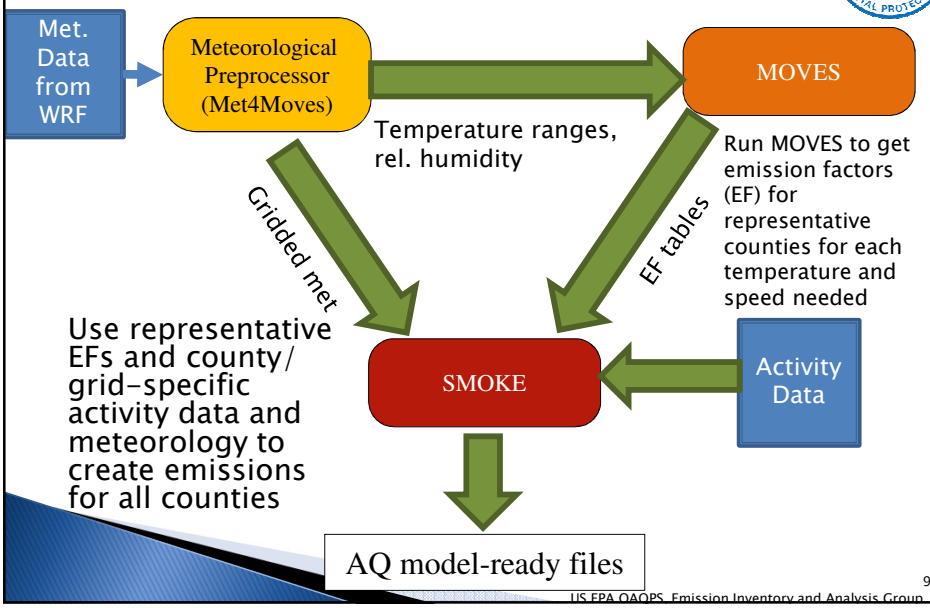
- Check SMOKE logs to ensure that all sources have references to VOC and PM speciation profiles.
- Sum model species to compare to VOC and PM2.5 inventory totals.
- Compare integrated species to inventory for full and partial integration sectors.
- Do a quick manual calculation of a species for a specific FIPS/SCC to ensure that the post-SMOKE value is using the correct profile (or profiles in the case of GSPRO_COMBO).
- Check SMOKE logs for warnings or errors. For example:
  - BAFM but no VOC for an integrate source
  - No TOG conversion factor
  - Skipping pollutant [X] for other than $PM_{10}$ and *_NOI pollutants
- Look at the output species to make sure all of the expected species are there for the specific mechanism (CB05 vs CB6 vs …).

# Questions?

- Any questions on speciation?

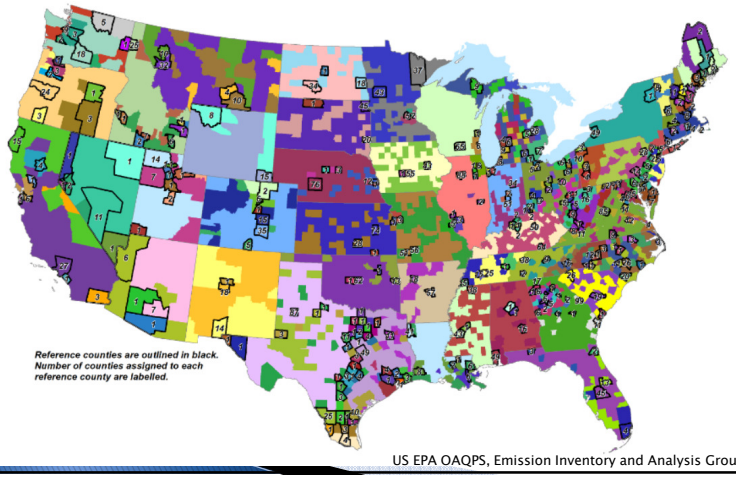


# Onroad Emissions Modeling



# Representative Counties

- 3000+ counties are mapped to approx. 300 representative counties according to: state, fuels, age distribution, ramp fraction, I/M programs, emissions standards



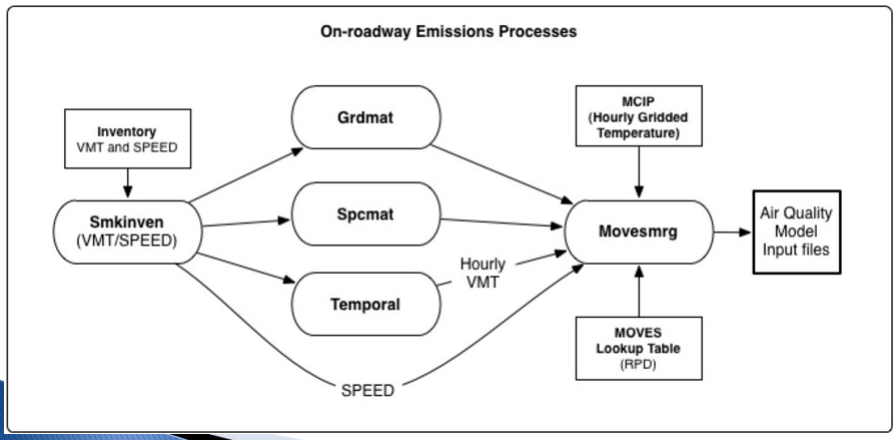



# Emission Processes in SMOKE/MOVES

- On-roadway emissions
  - Rate-per-distance (RPD)
  - Exhaust, evaporative, evaporative permeation, refueling, brake and tire wear
  - SMOKE uses: VMT, SPEED, speed profiles, and temperature T (gridded, hourly)
- Off-network (i.e. parked vehicles)
  - Rate-per-vehicle (RPV)
    - Exhaust, evaporative, evaporative permeation, refueling
    - SMOKE uses: VPOP and T (gridded, hourly)
  - Rate-per-profile (RPP)
    - Evaporative fuel vapor venting: hot soak (immediately after a trip) and diurnal (vehicle parked for a long period)
    - SMOKE uses: VPOP and T (gridded, daily min/max)
  - Rate-per-hour (RPH)
    - Hoteling: extended idle and auxiliary power units (APU)
    - SMOKE uses: Hoteling hours and T (gridded, hourly)

# On-roadway Processing (RPD)

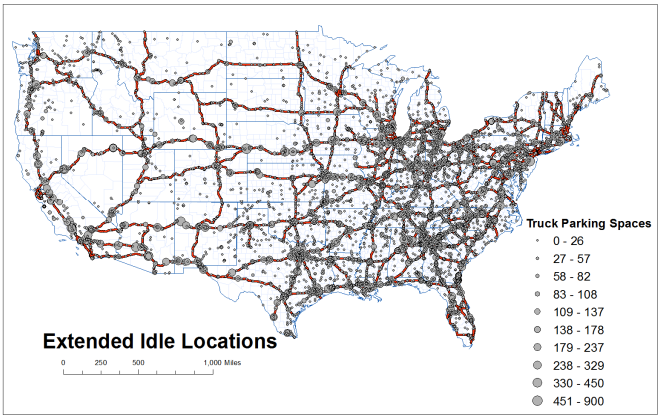
- Uses Standard SMOKE programs + Movesmrg
  - Input "inventory" is VMT and SPEED data




US EPA OAQPS, Emission Inventory and Analysis Group

# Onroad Hoteling

- Hoteling = Overnight truck idling: extended idle and APU
- States can submit hoteling hours by county
- EPA estimates use combination long-haul trucks VMT on restricted roads (urban + rural) to distribute hoteling hours
- Created temporal profile opposite of truck driving hours
- Spatial surrogate is based on truck parking spaces




98

# Recent Onroad Emissions Modeling Developments

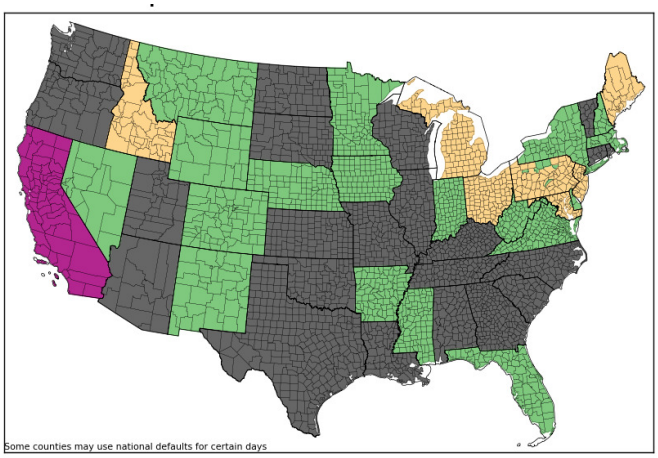
- SCCs used since 2011NEIv2 map to MOVES source types, road types, and aggregated processes
- Speciation is done in MOVES for CB05+CB6
- Long-haul vs short-haul splits are region-specific
- On-network spatial surrogates are based on VMT
- Many off-network surrogates are based on NLCD



# Onroad Temporal Profiles

- Temporal profiles based on 2012 Vehicle Travel Information System (VTRIS) data
  - Reported traffic count data to the Federal Highway Administration (FHWA)
  - Varies by state , HPMS vehicle (10, 20, 30, …) and road type
  - Distinct hourly / diurnal profiles for weekdays/Sat/Sunday
  - Day of the week profiles (i.e. Monday vs Tuesday vs …)
- Combined with more refined use of state submitted temporal information via NEI

# Temporal Profile Data Sources




VTRIS state

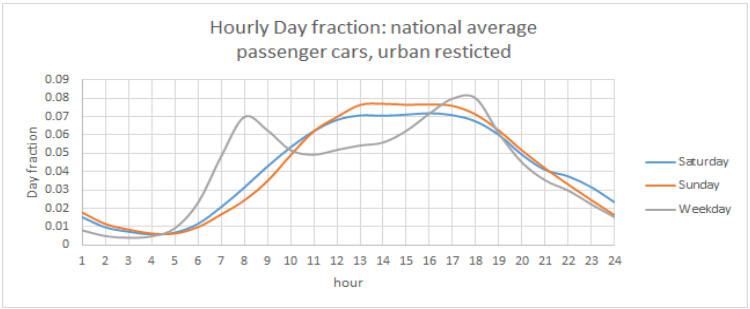
MOVES VMT

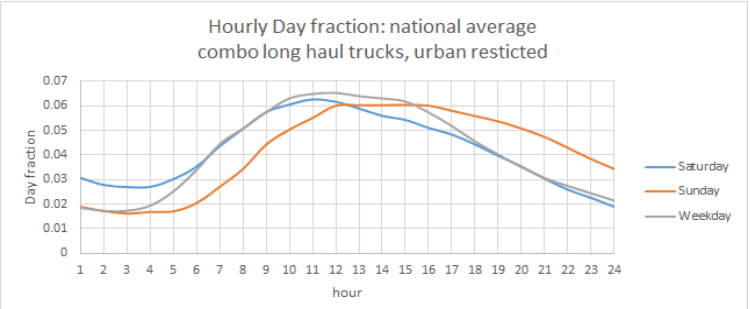
CARB

VTRIS/MOVES national average



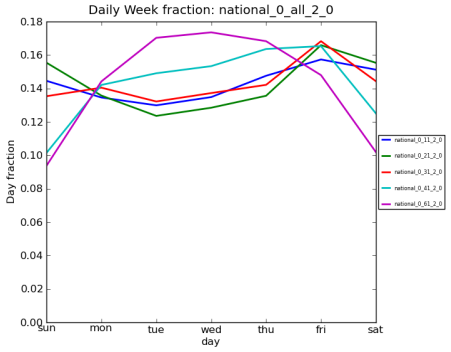
# National Default Diurnal Temporal Profiles

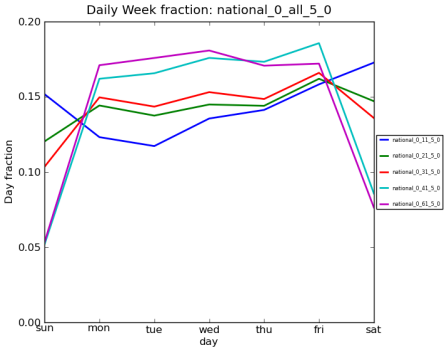


# National Day of Week Temporal Profiles

- Each color represents a different vehicle type
- Many states have state specific profiles



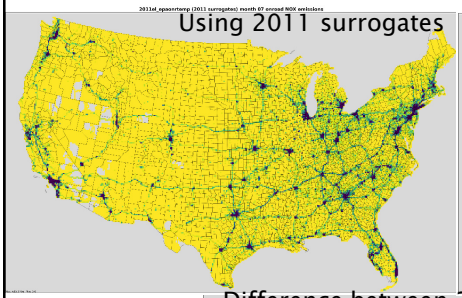

Rural restricted:
light-duty have Friday peak

Urban unrestricted:
more traffic weekdays

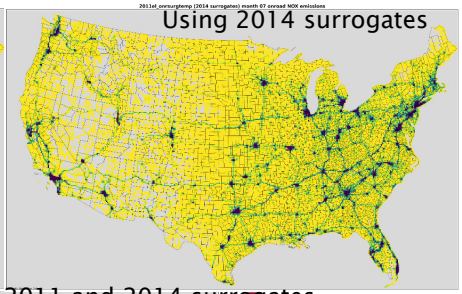


# Impacts of new Spatial Surrogates on 2011 Onroad NOx Emissions

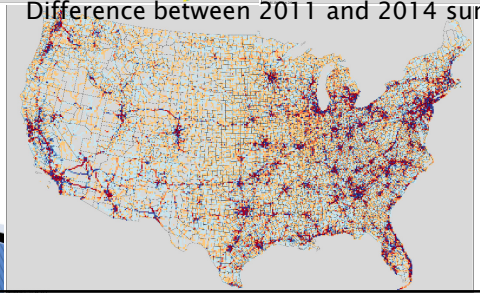
Using 2011 surrogates



Using 2014 surrogates



Difference between 2011 and 2014 surrogates



# Questions?

- Any questions on onroad emissions processing?



# Final Merging and QA

- After all sectors have been processed through SMOKE, the ground-level emissions are merged using the SectorMerge script
  - Key input file = Sector list file
- If CAMx is to be run instead of CMAQ, then need to run conversion scripts

# Sector List Input to Sector Merge Script – 2023el Case

| sector | sectorcase | Sectbaseyr | mrgapproach | prevyrspinup | endzip | mergesector |
|---|---|---|---|---|---|---|
| afdust_adj | 2023el_cb6v2_v6_11g | 2011 | all | SectBaseYr | Y | Y |
| ag | 2023el_cb6v2_v6_11g | 2011 | all | SectBaseYr | Y | Y |
| agfire | 2011ek_cb6v2_v6_11g | 2011 | week_Y | SectBaseYr | N | Y |
| nonroad | 2023el_cb6v2_v6_11g | 2011 | mwdss_Y | SectBaseYr | N | Y |
| rail | 2023el_cb6v2_v6_11g | 2011 | aveday_N | SectBaseYr | N | Y |
| nonpt | 2023el_cb6v2_v6_11g | 2011 | week_Y | SectBaseYr | N | Y |
| np_oilgas | 2023el_cb6v2_v6_11g | 2011 | week_Y | SectBaseYr | N | Y |
| rwc | 2023el_cb6v2_v6_11g | 2011 | all | SectBaseYr | Y | Y |
| ptegu | 2023el_cb6v2_v6_11g | 2011 | all | SectBaseYr | Y | Y |
| ptnonipm | 2023el_cb6v2_v6_11g | 2011 | mwdss_Y | SectBaseYr | N | Y |
| pt_oilgas | 2023el_cb6v2_v6_11g | 2011 | mwdss_Y | SectBaseYr | N | Y |
| ptfire | 2011ek_cb6v2_v6_11g | 2011 | all | SectBaseYr | Y | N |
| othafdust_adj | 2011ek_cb6v2_v6_11g | 2011 | all | SectBaseYr | N | Y |
| beis | 2011ek_cb6v2_v6_11g | 2011 | all | actualMet | N | Y |
| cmv | 2023el_cb6v2_v6_11g | 2011 | aveday_N | SectBaseYr | N | Y |
| ptfire_mxca3D | 2011el_cb6v2_v6_11g | 2011 | all | SectBaseYr | Y | N |
| onroad | 2023el_cb6v2_v6_11g | 2011 | all | SectBaseYr | Y | Y |
| onroad_catx_adj | 2023el_cb6v2_v6_11g | 2011 | all | SectBaseYr | Y | Y |
| othar | 2023el_cb6v2_v6_11g | 2011 | week_N | SectBaseYr | N | Y |
| othon | 2023el_cb6v2_v6_11g | 2011 | week_N | SectBaseYr | N | Y |
| othpt | 2023el_cb6v2_v6_11g | 2011 | mwdss_N | SectBaseYr | N | N |



# Ramp-up Period

- For regional CAP-focused modeling, we typically have a ramp-up period of 10 days (i.e., starting on December 22 of the previous year)
  - For most sectors, emissions from December of the modeled year are repeated during the ramp-up
  - For biogenic emissions, data based on actual prior year meteorology are used
- For hemispheric modeling, the ramp-up is longer – approx. four months
  - Prior year fire emissions used for ramp-up

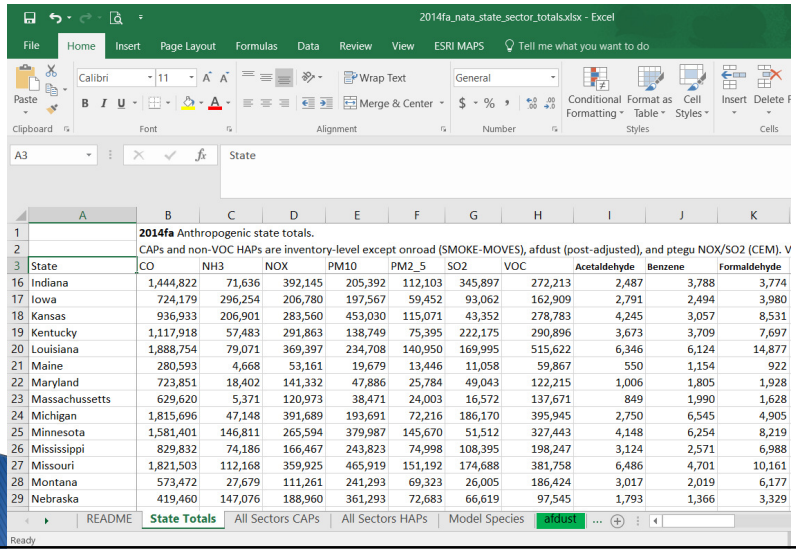
# QA of Merged Emissions

- Look at the mrggrid logs to ensure that the correct case/sector files are merging and all sectors with ground-level emissions are included
- Generate domain totals of the 2D and inline files and compare back to the sum of the sector SMOKE annual reports.
- Check the size of the 2D merged emissions files to make sure that the file size is the same for each day (corrupted files will be smaller)
- Sometimes compare day-specific or annual total gridded emissions to a previous run



# State-Sector Totals Report

- State totals by sector before and after SMOKE



2014fa_nata_state_sector_totals.xlsx - Excel

**2014fa** Anthropogenic state totals.

CAPs and non-VOC HAPs are inventory-level except onroad (SMOKE-MOVES), afdust (post-adjusted), and ptegu NOX/SO2 (CEM). V

| State | CO | NH3 | NOX | PM10 | PM2_5 | SO2 | VOC | Acetaldehyde | Benzene | Formaldehyde |
|---|---|---|---|---|---|---|---|---|---|---|
| Indiana | 1,444,822 | 71,636 | 392,145 | 205,392 | 112,103 | 345,897 | 272,213 | 2,487 | 3,788 | 3,774 |
| Iowa | 724,179 | 296,254 | 206,780 | 197,567 | 59,452 | 93,062 | 162,909 | 2,791 | 2,494 | 3,980 |
| Kansas | 936,933 | 206,901 | 283,560 | 453,030 | 115,071 | 43,352 | 278,783 | 4,245 | 3,057 | 8,531 |
| Kentucky | 1,117,918 | 57,483 | 291,863 | 138,749 | 75,395 | 222,175 | 290,896 | 3,673 | 3,709 | 7,697 |
| Louisiana | 1,888,754 | 79,071 | 369,397 | 234,708 | 140,950 | 169,995 | 515,622 | 6,346 | 6,124 | 14,877 |
| Maine | 280,593 | 4,668 | 53,161 | 19,679 | 13,446 | 11,058 | 59,867 | 550 | 1,154 | 922 |
| Maryland | 723,851 | 18,402 | 141,332 | 47,886 | 25,784 | 49,043 | 122,215 | 1,006 | 1,805 | 1,928 |
| Massachussetts | 629,620 | 5,371 | 120,973 | 38,471 | 24,003 | 16,572 | 137,671 | 849 | 1,990 | 1,628 |
| Michigan | 1,815,696 | 47,148 | 391,689 | 193,691 | 72,216 | 186,170 | 395,945 | 2,750 | 6,545 | 4,905 |
| Minnesota | 1,581,401 | 146,811 | 265,594 | 379,987 | 145,670 | 51,512 | 327,443 | 4,148 | 6,254 | 8,219 |
| Mississippi | 829,832 | 74,186 | 166,467 | 243,823 | 74,998 | 108,395 | 198,247 | 3,124 | 2,571 | 6,988 |
| Missouri | 1,821,503 | 112,168 | 359,925 | 465,919 | 151,192 | 174,688 | 381,758 | 6,486 | 4,701 | 10,161 |
| Montana | 573,472 | 27,679 | 111,261 | 241,293 | 69,323 | 26,005 | 186,424 | 3,017 | 2,019 | 6,177 |
| Nebraska | 419,460 | 147,076 | 188,960 | 361,293 | 72,683 | 66,619 | 97,545 | 1,793 | 1,366 | 3,329 |

README | State Totals | All Sectors CAPs | All Sectors HAPs | Model Species | afdust

# CAMx Conversion

- EPA always prepares the emissions files initially using CMAQ's netCDF format
- Scripts are provided to convert to CAMx:
  - Species are mapped from CMAQ model ready species names to CAMx names
  - Merged gridded 2D emissions are converted from IOAPI format to CAMx model ready format "emis2d" files
  - Gridded CAMx emissions are merged with land use and met-based surf zone sea-salt emissions files
  - Inline CMAQ model ready emissions are converted to CAMx point "ptsr" emissions for each sector
    - This step requires that fires have been processed in 3D
  - The CAMx point "ptsr" emissions are merged into a single point "mrgpt" file for the CAMx model



# Source apportionment

- Source apportionment is used for transport analyses
  - Evaluate significant contribution by states
  - Understand which sectors contribute to AQ issues
- Source apportionment requires that all sectors have been tagged and written as CAMX ptsr emissions files
- For most sectors, SMOKE can prepare both SA and non-SA outputs simultaneously
  - Onroad for SA takes a lot of RAM and we run in shorter time chunks than our typical 7 days
- Scripts are available for SA configuration
- A standalone 2-D sea-salt file is read by CAMx (all others are in CAMx ptsr format)

# Emissions Modeling Software and Data

- The CMAS Center (https://www.cmascenter.org/) distributes SMOKE, CMAQ, VERDI, the Surrogate Tool, Spatial Allocator, Speciation Tool, and the Control Strategy Tool which includes the Emissions Modeling Framework
- SMOKE software and documentation is available from http://www.cmascenter.org/smoke
  - SMOKE 4.0 has support for hemispheric modeling
  - SMOKE 4.5 has support for preparing emissions for AERMOD modeling
- A WIKI for SMOKE that answers common questions about emissions modeling is here: https://www.airqualitymodeling.org/index.php
- EPA's emissions modeling platform data, scripts, and documentation are available from https://www.epa.gov/air-emissions-modeling



# Questions?

- Any final questions on the base year part of the training?
- Contacts: eyth.alison@epa.gov, Vukovich.jeffrey@epa.gov