Emissions Inventory Preparation for Air Quality Modeling (Base Year)

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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 the process of emissions modeling

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 Source Processing
- 11:45 Final merging, conversion, and QA
- 12:00 LUNCH

Background: Purpose and Contents of a Modeling Platform

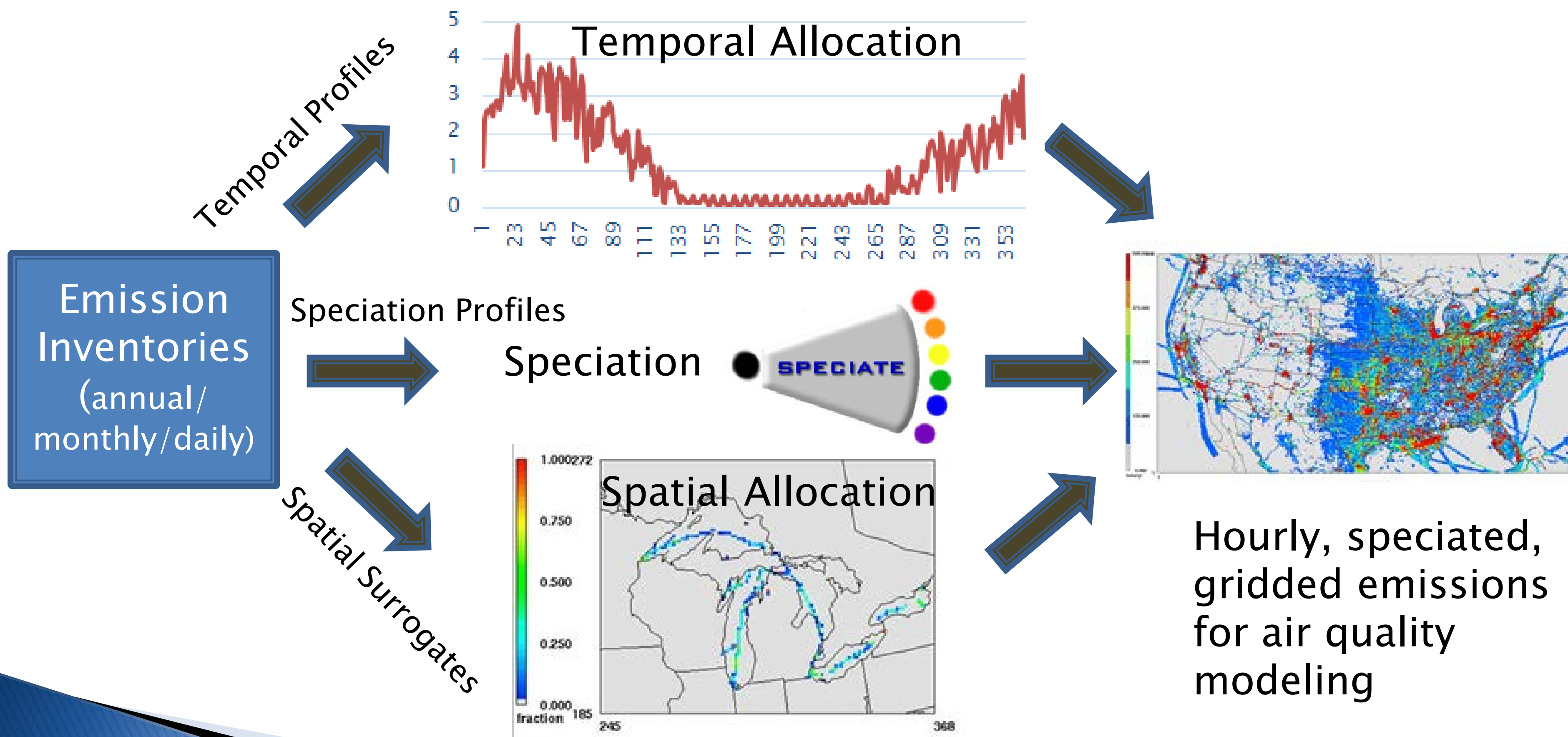
- A modeling platform provides a comprehensive air quality modeling system that uses the most recent technically sound data and state-of-the-science tools available
- Modeling platforms are used to support EPA regulations and other analyses
- Major components of a modeling platform:
  - Meteorological 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/or temporalization (e.g., onroad mobile, biogenic, res. wood combustion, 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

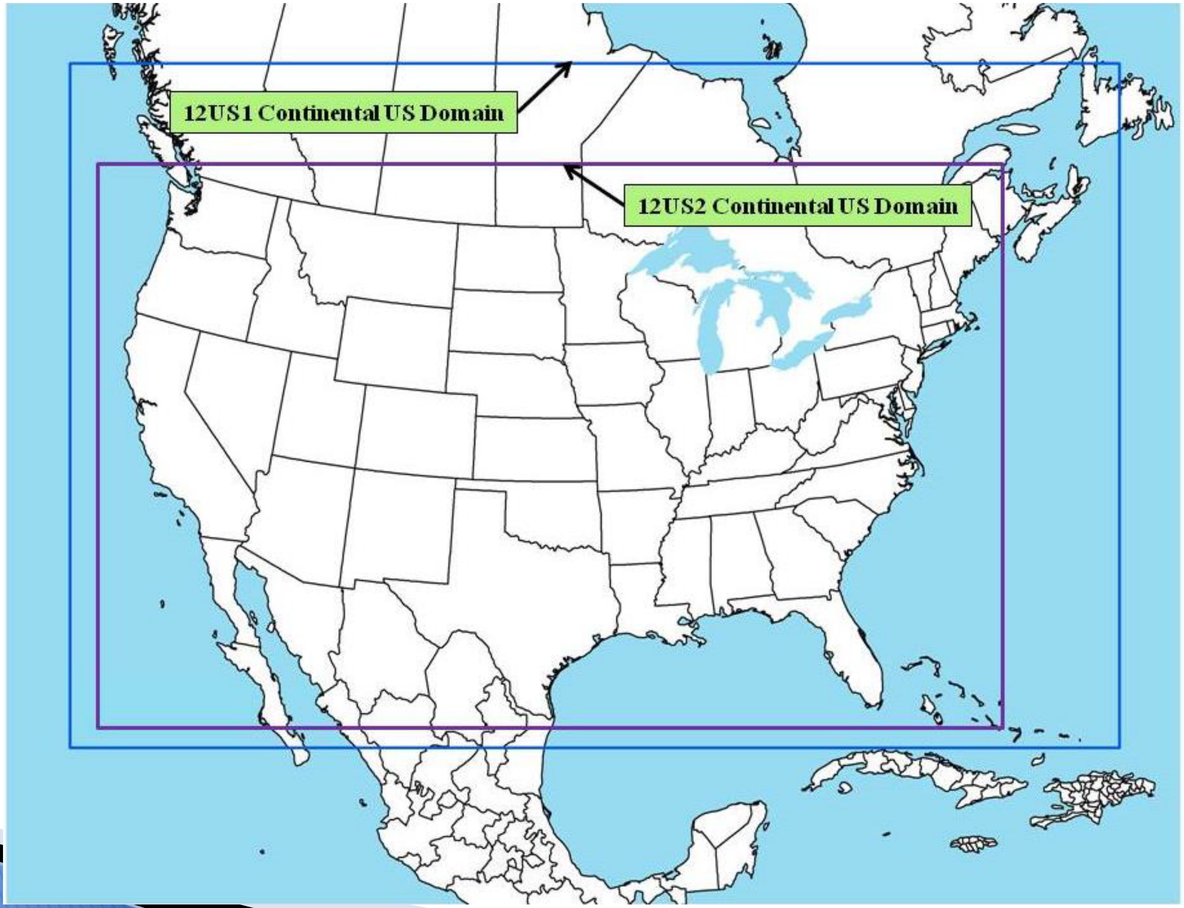
- 2011v6.3 platform is based on 2011NEIv2
  - First number (2011) is the base year being modeled
  - The number before the "." (6) corresponds to a specific NEI year (e.g., 6 means 2011 NEI was used)
  - The number after the "." (3) is an iteration of the platform (e.g., 3 is a third major iteration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

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 emissions case configuration, cb6v2 = CB6 speciation, v6 = platform, 11g = WRF 3.5 for 2011
  - **2016fc_cb6camx_16j**: 2016 = year modeled, f = 2014 NEI, c = third case, cb6camx = CB6 speciation, 16j = WRF 3.8 for 2016

EPA US 12km Modeling Platform Domains

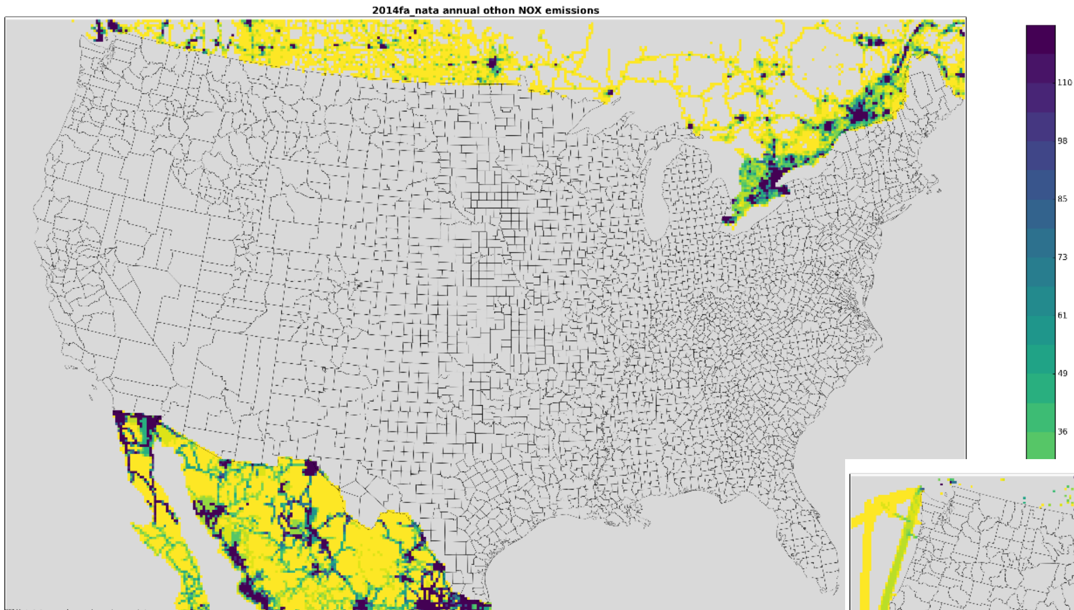
- US domains / grids use consistent map projections (Lambert)
- Other domains also exist (e.g., 36km, 4km, hemispheric)
- Many US domains include parts of Canada and/or Mexico



Non-US emissions in the Emissions Modeling Platforms

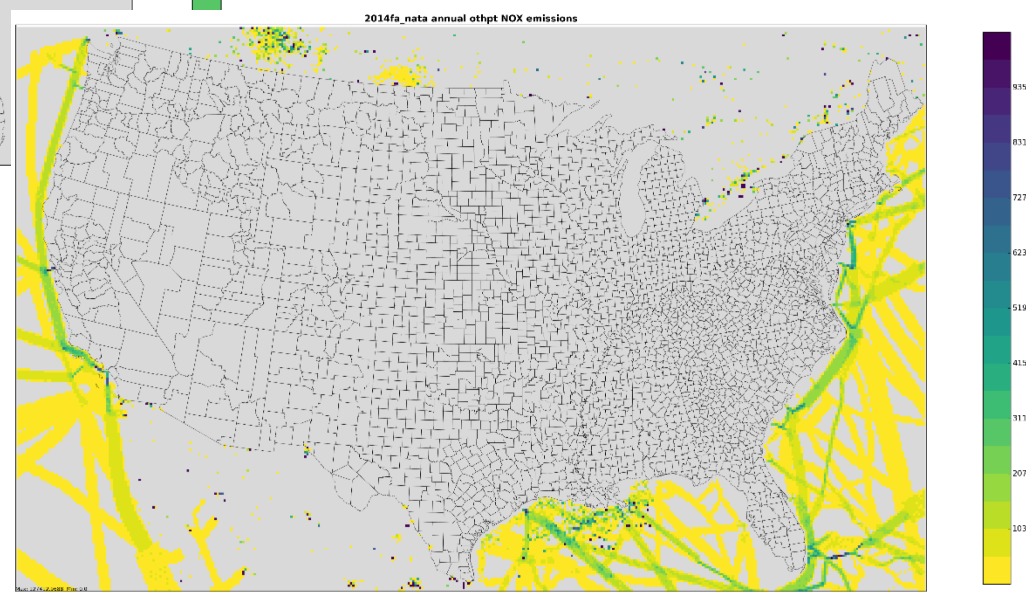
- Canada emissions & ancillary data (e.g., surrogates)
  - Courtesy Environment Canada
  - 2010 used until 2013 data provided in spring of 2017
  - Fire emissions provided for summer 2011 and other recent years
- Mexico 2008 emissions and projections of these
  - Based on Inventario Nacional de Emisiones 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 in Canada for winter]
- 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 inventory or processing characteristics and starts with lowercase letter
- Specific sectors vary by modeling platform version 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 at the end merges the ground-level emissions for a case together**

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 to a previous platform**
  - Create difference reports by state, county, and/or SCC
  - Create charts and maps
  - Make sure any changes make sense
- Update ancillary files to account for new SCCs and data

Quality Assurance Examples

- We perform QA for each part of the emissions modeling process
- Examples of QA assessments
  - Inventory comparisons (new vs old)
  - Temporal allocation: Sub-annual (e.g. ozone season, hourly, daily)
  - Speciation: Examine speciated PM or VOC
  - Spatial Allocation: Review gridded inventory emissions
- Some examples of typical QA products follow

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%

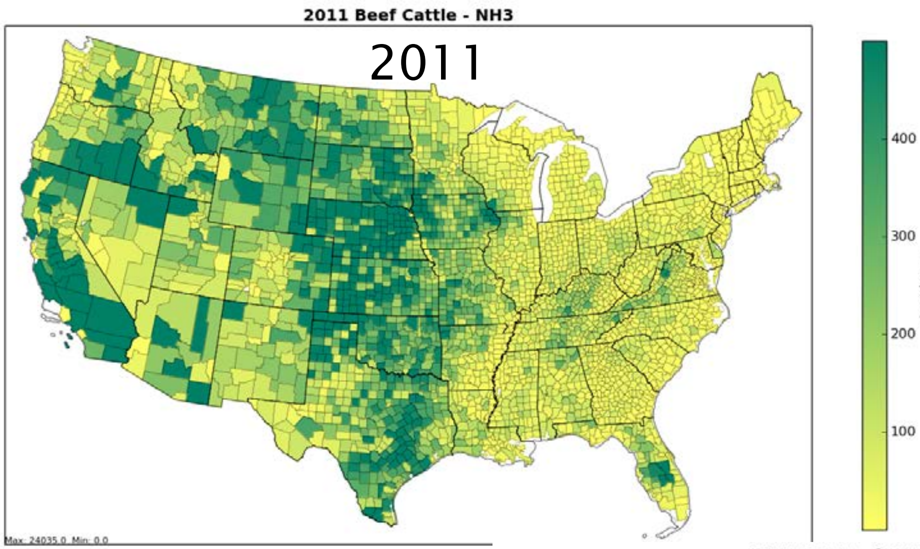
2014 vs 2016 County-level Comparisons

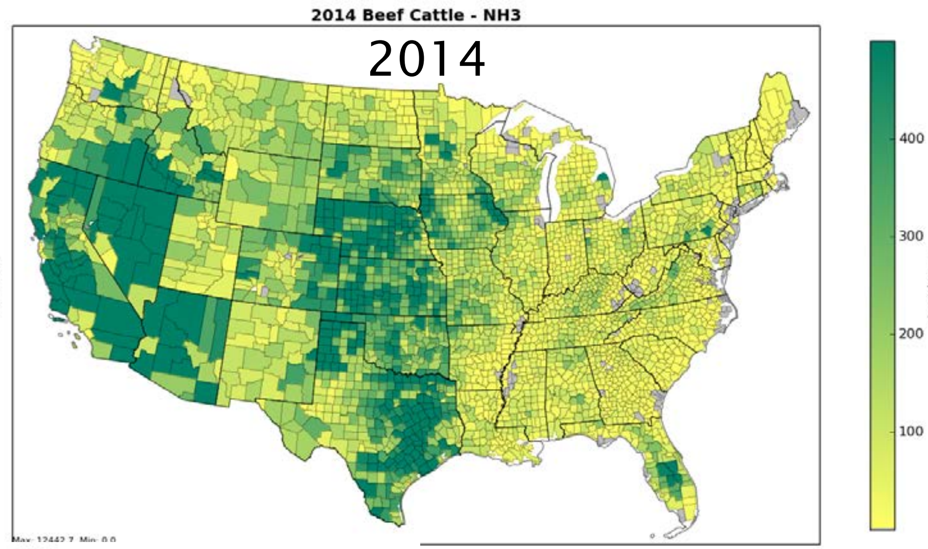
sector	state	county	poll	ann_emis_2014fb	ann_emis_2016fc	diff	pdiff
beis	Alabama	Autauga Co	CO	2,458	2,756	298	12.1%
beis	Alabama	Autauga Co	NOX	157	167	10	6.2%
beis	Alabama	Autauga Co	VOC_INV	21,332	23,829	2,496	11.7%
beis	Alabama	Baldwin Co	CO	7,276	8,206	930	12.8%
beis	Alabama	Baldwin Co	NOX	399	433	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

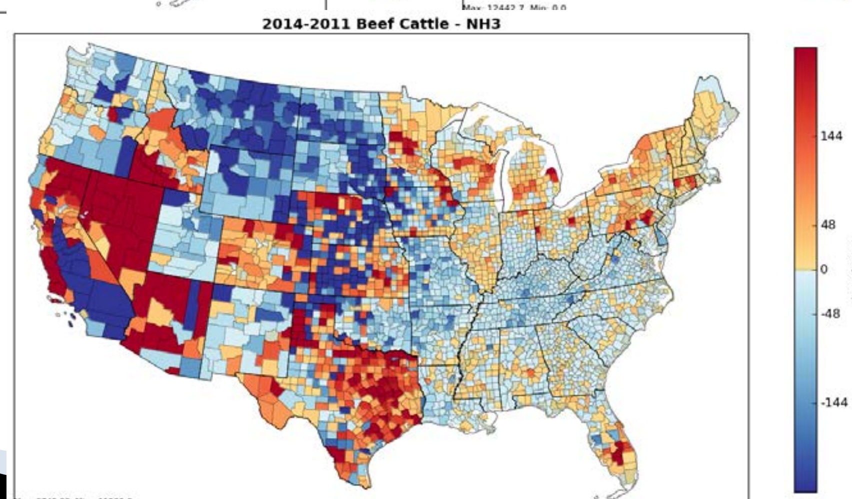
sector	state	county	poll	ann_emis_2014fb	ann_emis_2016fc	diff	pdiff
ptnonipm	Alabama	Autauga Co	CO	2,475	2,482	7	0.3%
ptnonipm	Alabama	Autauga Co	NH3	71	72	0	0.3%
ptnonipm	Alabama	Autauga Co	NOX	2,530	2,537	7	0.3%
ptnonipm	Alabama	Autauga Co	PM10	536	538	1	0.3%
ptnonipm	Alabama	Autauga Co	PM2_5	428	429	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





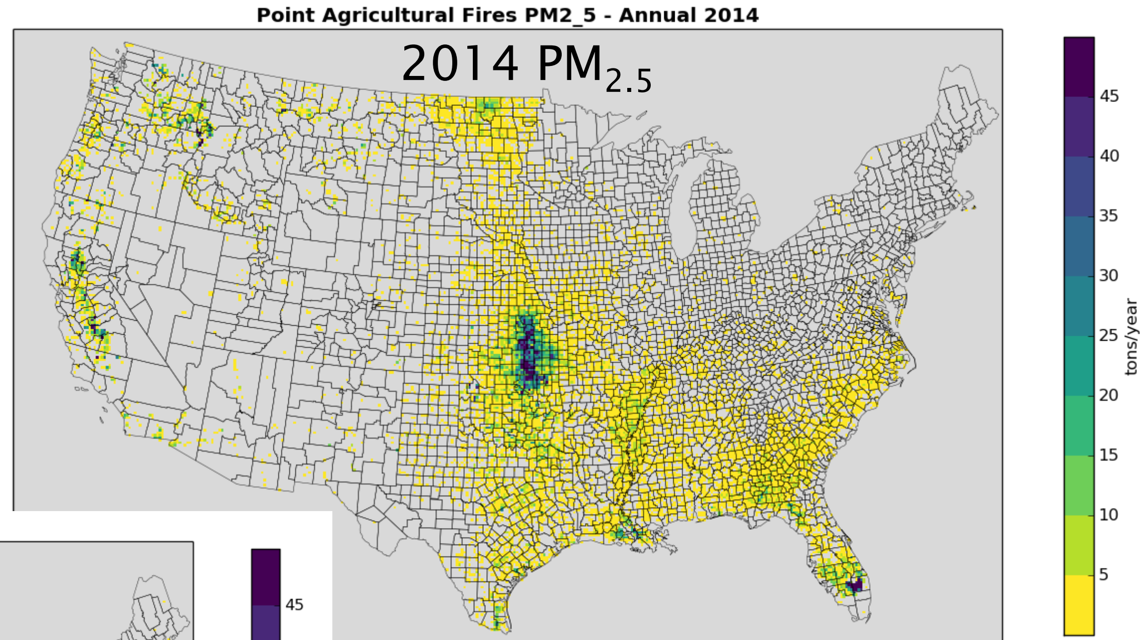
Maps help us see spatial variation and hot spots

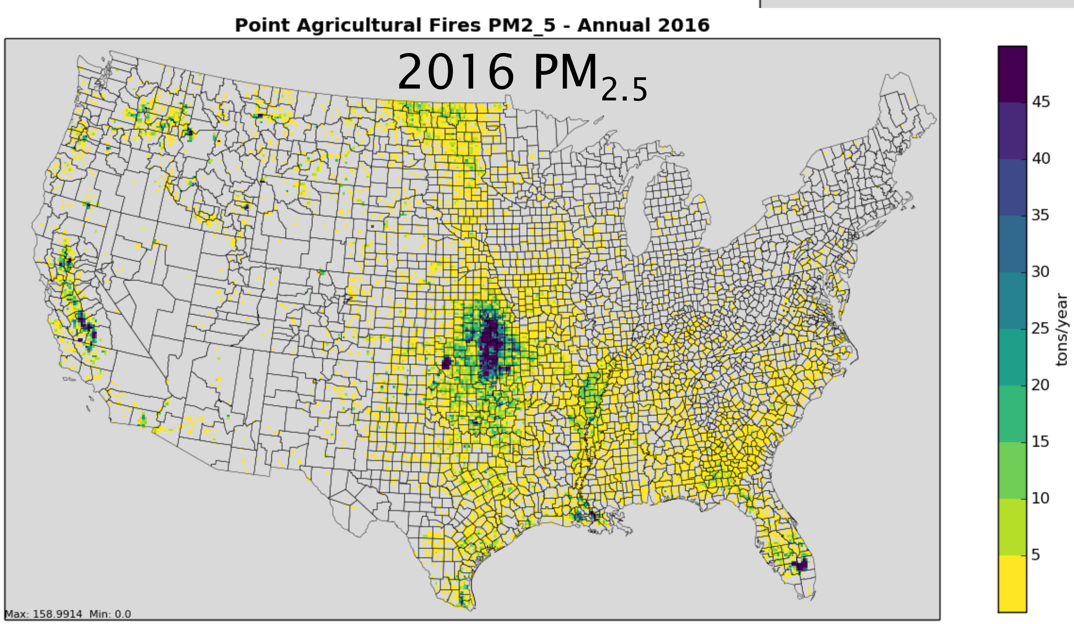


Most of our county-level maps are created with Python

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

- Most modeling platform inventories are the same as what is in the NEI, but some are not
  - 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

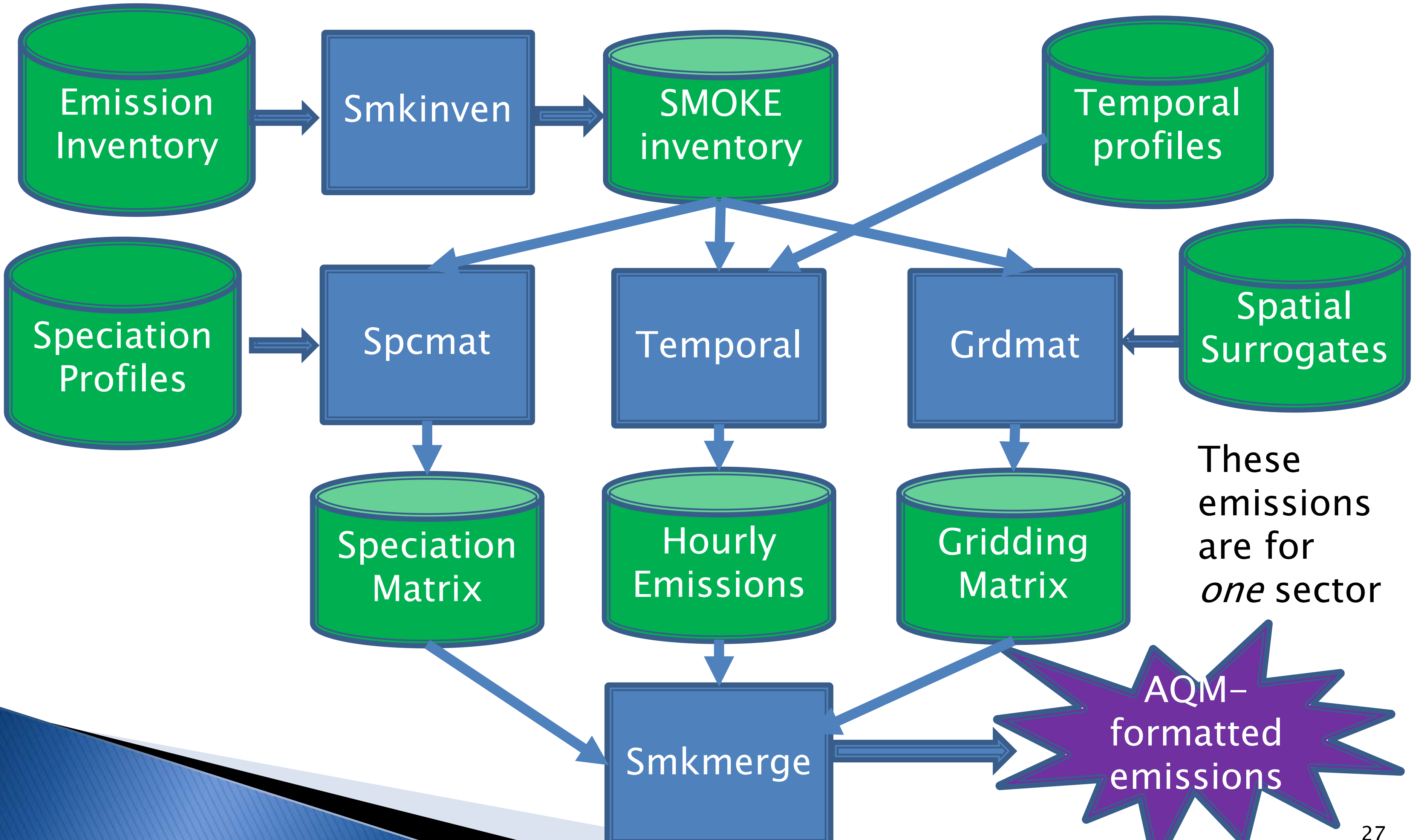
Questions?

- 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

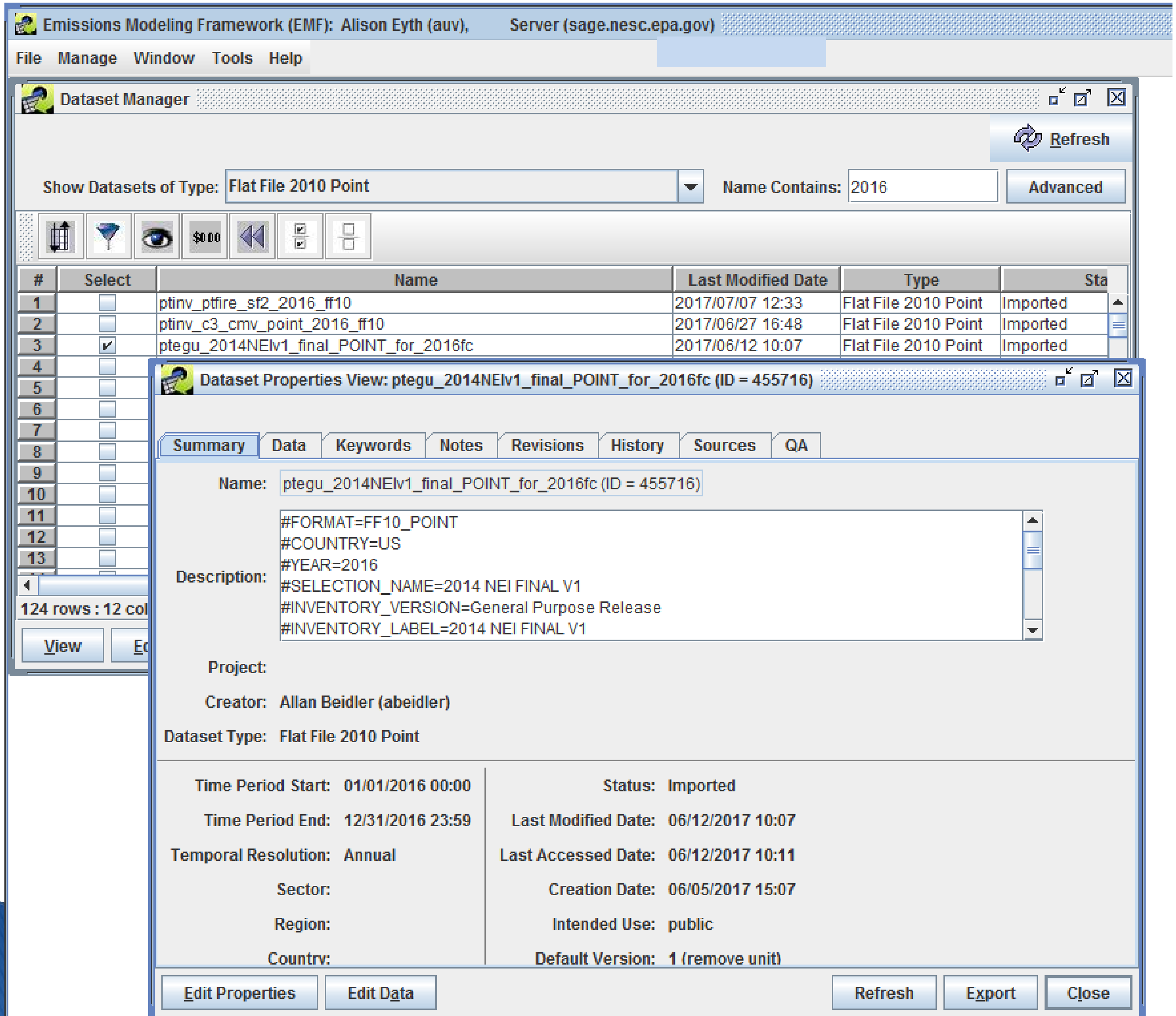
Special Emissions Models

- **<u>Biogenic Emission Inventory System (BEIS):</u>** part of SMOKE and CMAQ that creates air quality model-ready biogenic emissions
  - SMOKE programs: Normbeis3, Tmpbeis3
- **<u>Motor Vehicle Emission Simulator (MOVES)</u>**:
  - 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

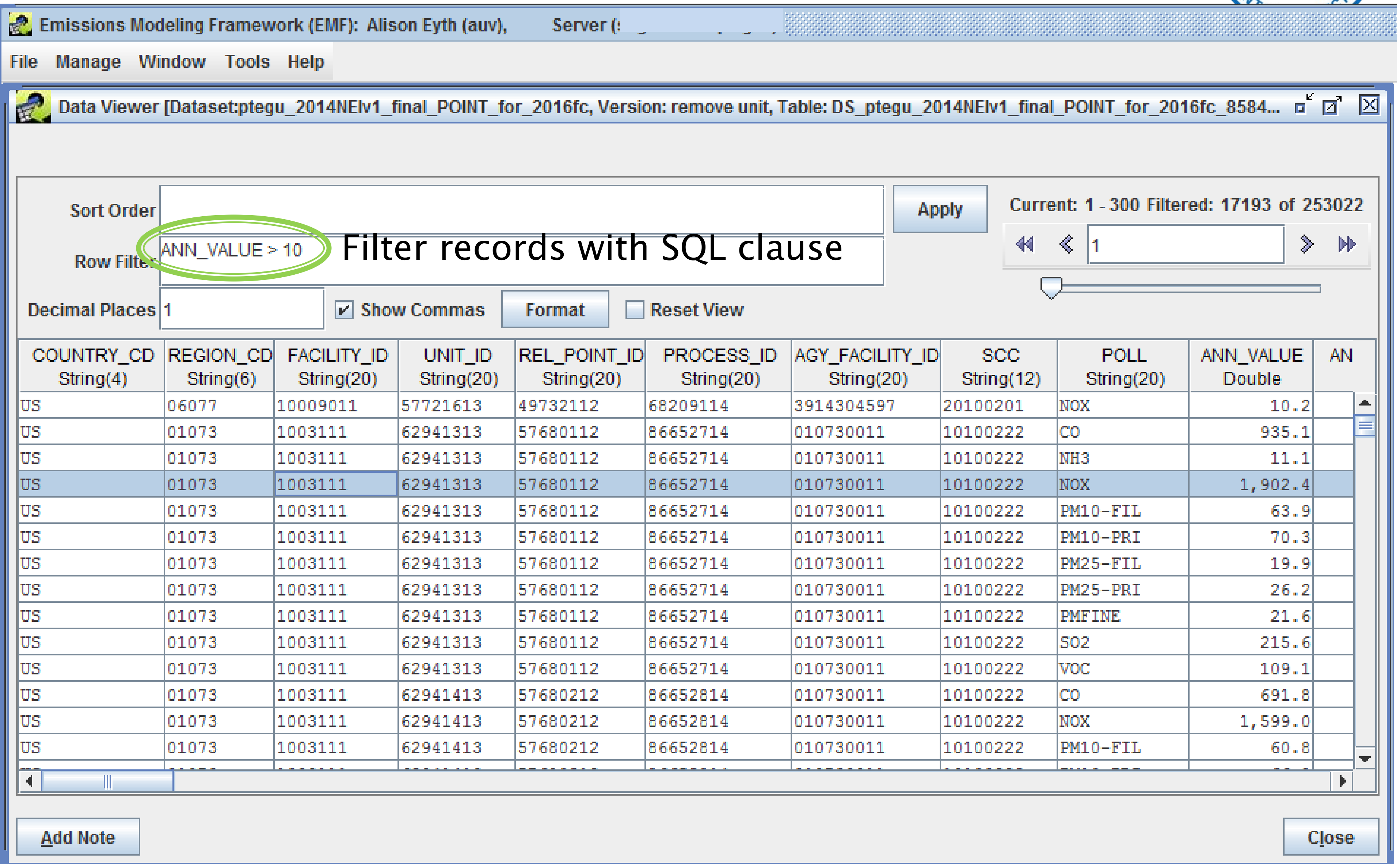
- Surrogate Tool: creates spatial surrogates from Shapefiles to put emissions into grid cells
- Speciation Tool: creates chemical speciation profiles from SPECIATE database profiles (e.g., NOx->NO+ NO_2, PM2.5->EC+OC+..., VOC->…)
- Gentpro: SMOKE program that creates meteorology-based temporal profiles
- 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 a Point Inventory



COUNTRY_CD String(4)	REGION_CD String(6)	FACILITY_ID String(20)	UNIT_ID String(20)	REL_POINT_ID String(20)	PROCESS_ID String(20)	AGY_FACILITY_ID String(20)	SCC String(12)	POLL String(20)	ANN_VALUE Double	AN
US	06077	10009011	57721613	49732112	68209114	3914304597	20100201	NOX	10.2	
US	01073	1003111	62941313	57680112	86652714	010730011	10100222	CO	935.1	
US	01073	1003111	62941313	57680112	86652714	010730011	10100222	NH3	11.1	
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US	01073	1003111	62941313	57680112	86652714	010730011	10100222	PM10-PRI	70.3	
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US	01073	1003111	62941313	57680112	86652714	010730011	10100222	PM25-PRI	26.2	
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US	01073	1003111	62941413	57680212	86652814	010730011	10100222	PM10-FIL	60.8	

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)

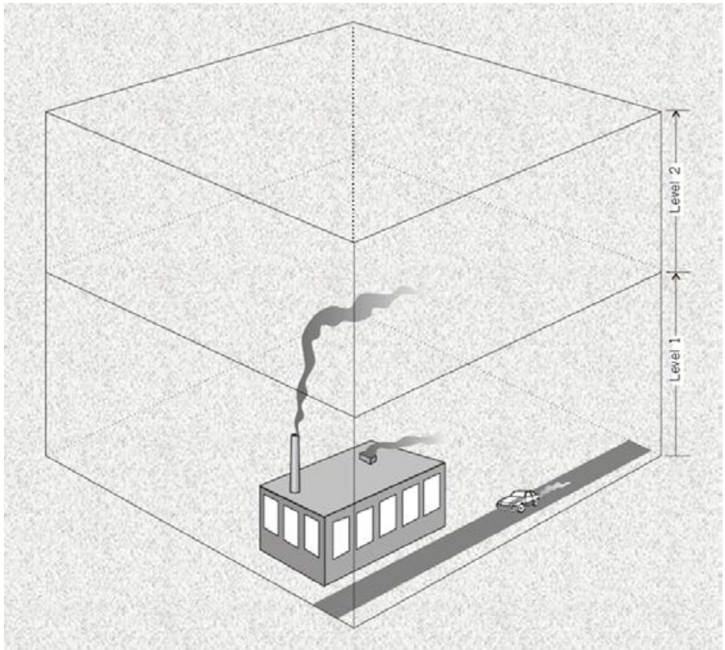
Platform sector	Spatial	Speciation	Inventory resolution	Plume rise
othafdust	Surrogates	Yes	annual	
othar	Surrogates	Yes	annual	
othpt	Point	Yes	annual	in-line*
ptfire_mxca	Point	Yes	daily	In-line
pt_oilgas	Point	Yes	annual	in-line
ptegu	Point	Yes	annual & hourly CEMS	in-line
ptfire	Point	Yes	daily	in-line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

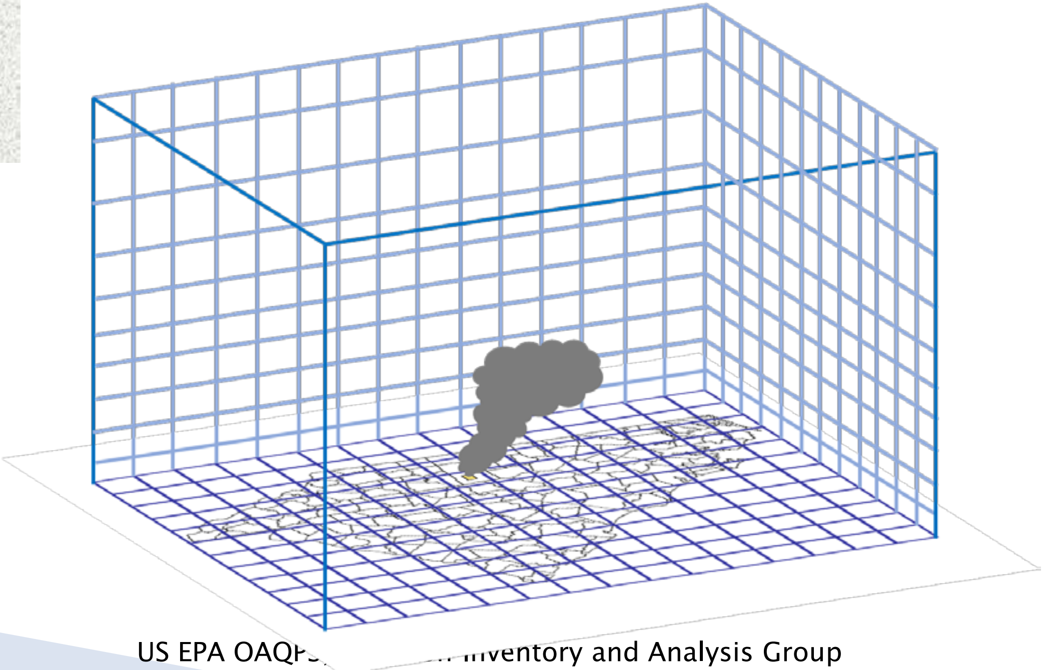
* in-line means it can be done in CMAQ

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: Vertical allocation





Plume Rise Formula

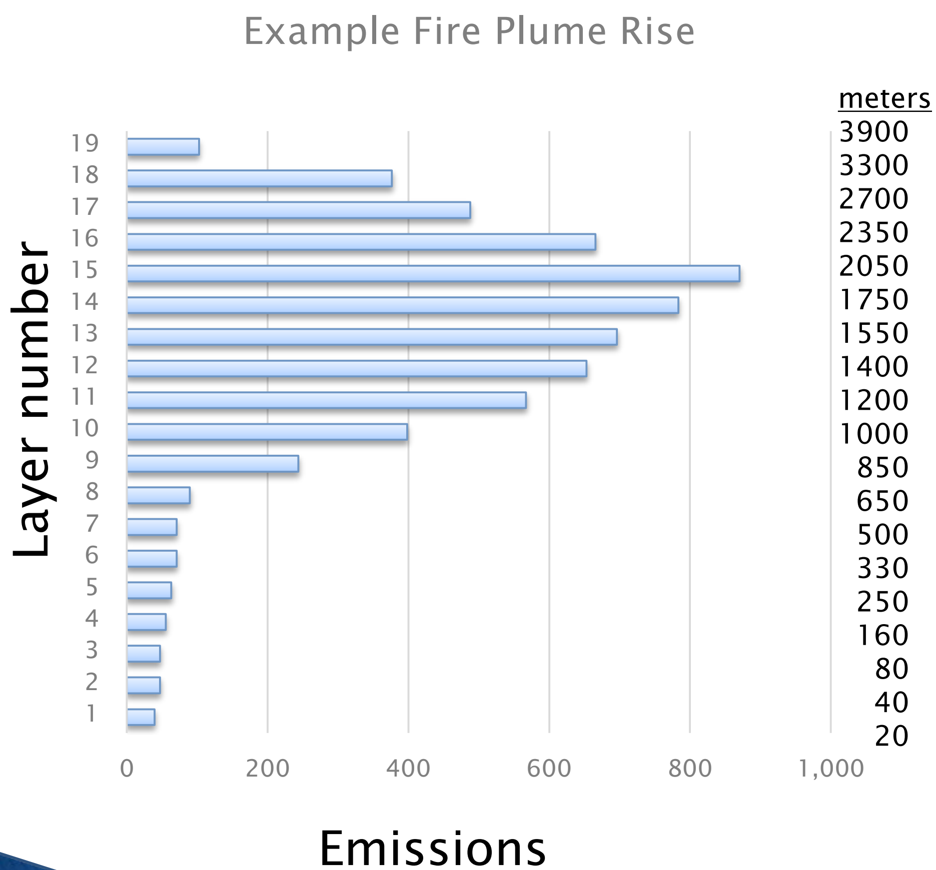
- **Stack parameters** for point sources affect plume rise
  - Height, diameter, velocity / flow, temperature

- **$F = 0.25 \times G \times V_S \times D_S^2 \times (T_S - T)/T_S$**
- 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



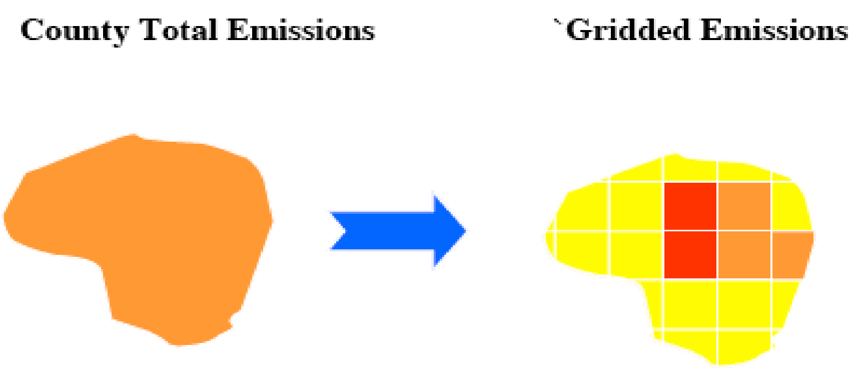
Questions?

- 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)

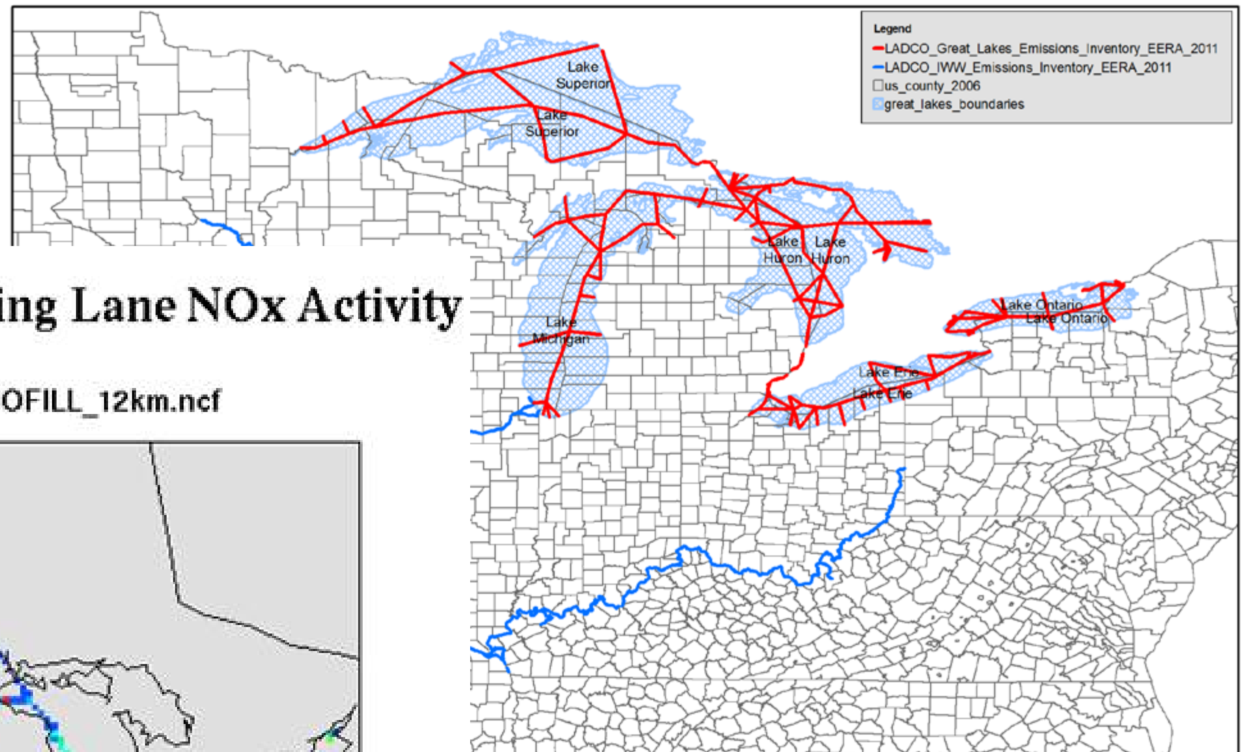


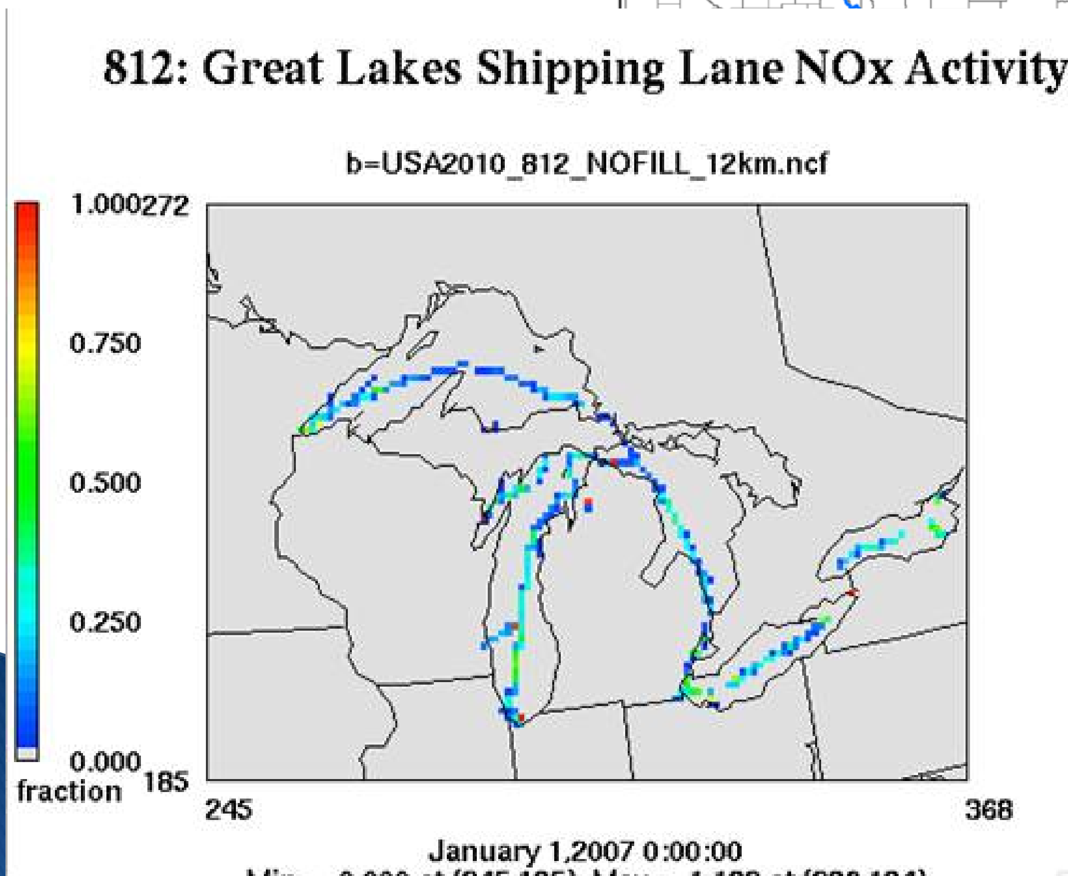
Data Used to Create a Spatial Surrogate with Surrogate Tool

- 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

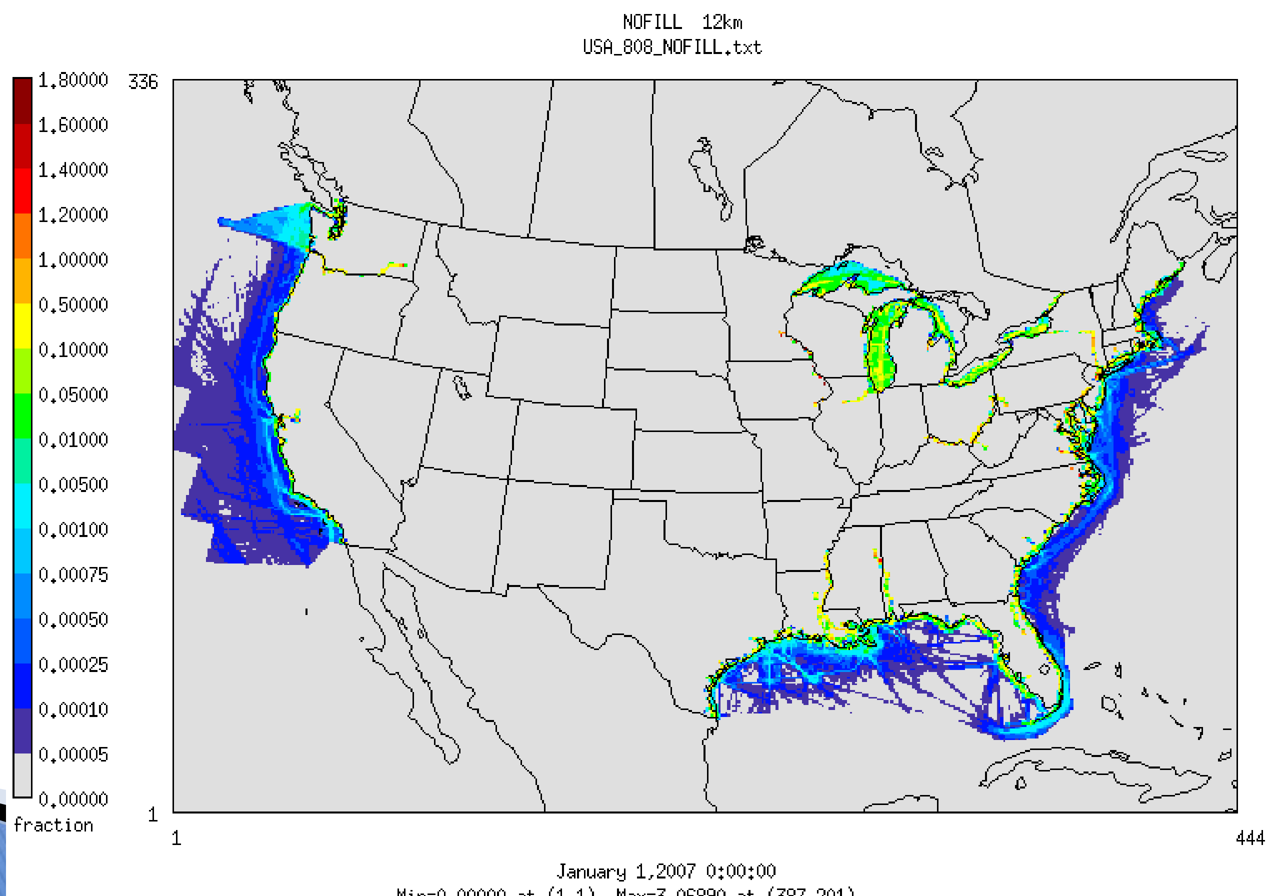
Data = US counties
Weight = NOx emissions
on shipping lanes
Output is US 12km grid





Alternative CMV Surrogate

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



Spatial Surrogate values

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

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

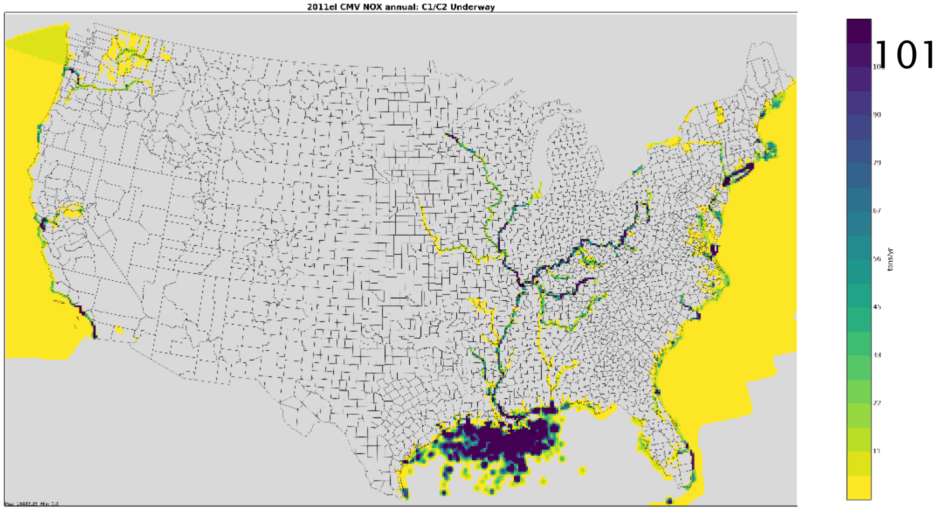
Sector	ID	Description	NH3	NOX	PM2_5	VOC
ag	310	NLCD Total Agriculture	3,135,285			
onroad	307	NLCD All Development		560,112	12,560	1,142,592
onroad	222	Urban Unrestricted AADT	42,001	1,223,593	54,345	376,209
nonpt	306	NLCD Med + High	22,268	239,863	290,187	864,662
onroad	232	Rural Unrestricted AADT	25,027	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

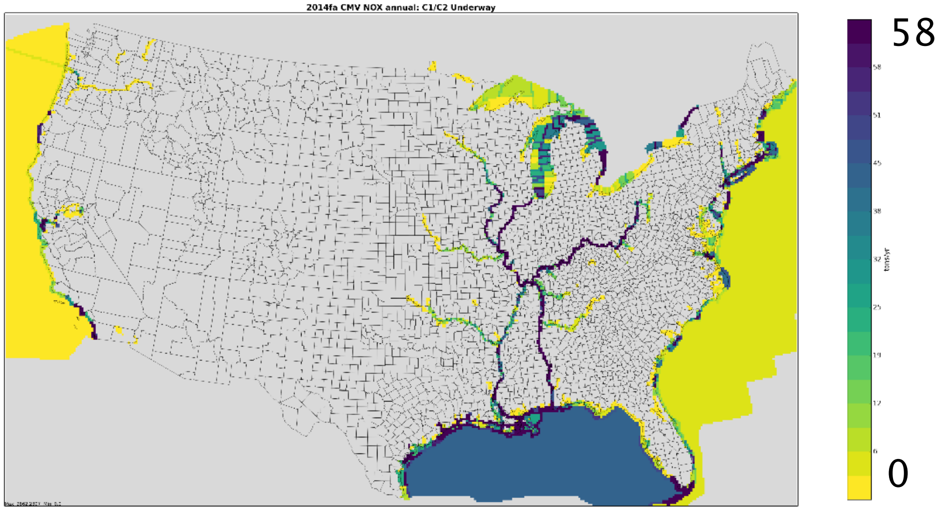
- Check SMOKE logs to ensure all sources have reference to spatial allocation profiles and only emissions outside the domain are not allocated.
- Review gridded emission plots by sector to ensure spatial patterns are reasonable (US sources are all in US, onshore emissions are all on land)
- Check inventory 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.

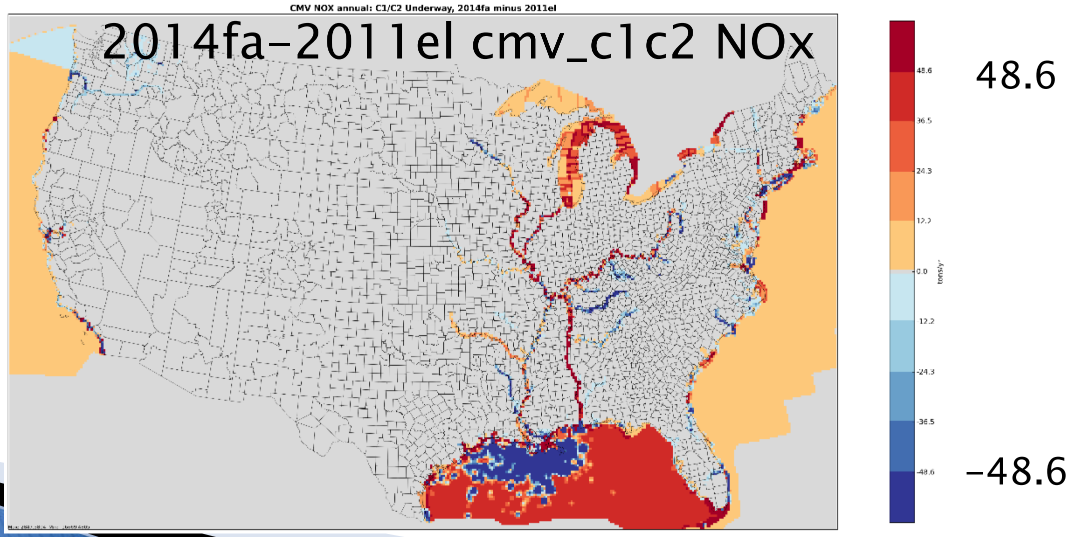
Maps Help us to Check Spatial Surrogates: cmv_c1c2 Example

2011el cmv_c1c2 NOx



2014fa cmv_c1c2 NOx





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

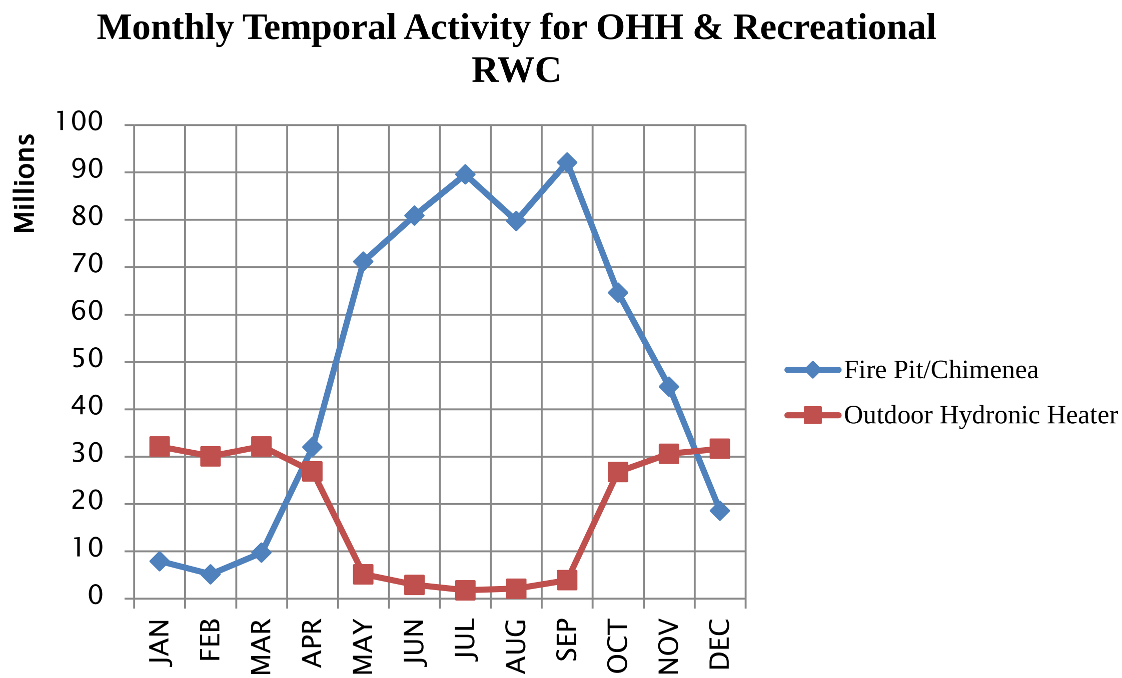
Questions?

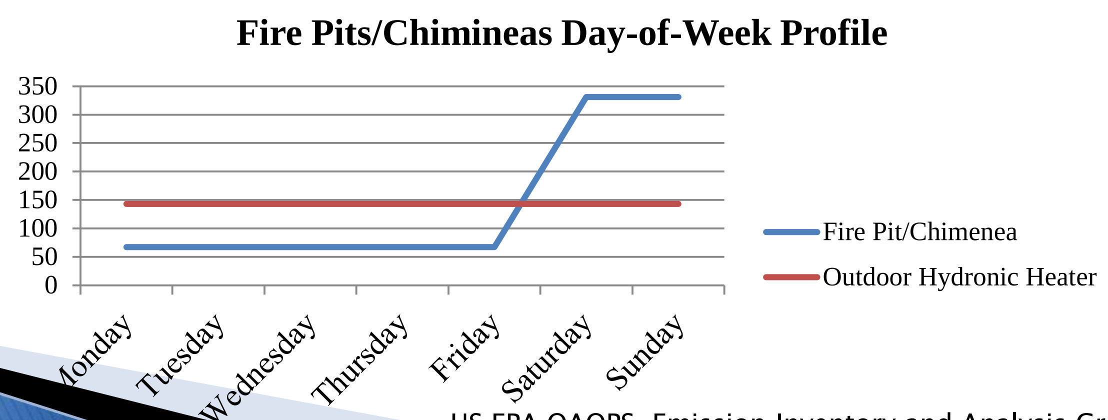
- In this section we've covered some details on spatial allocation

Temporal Allocation

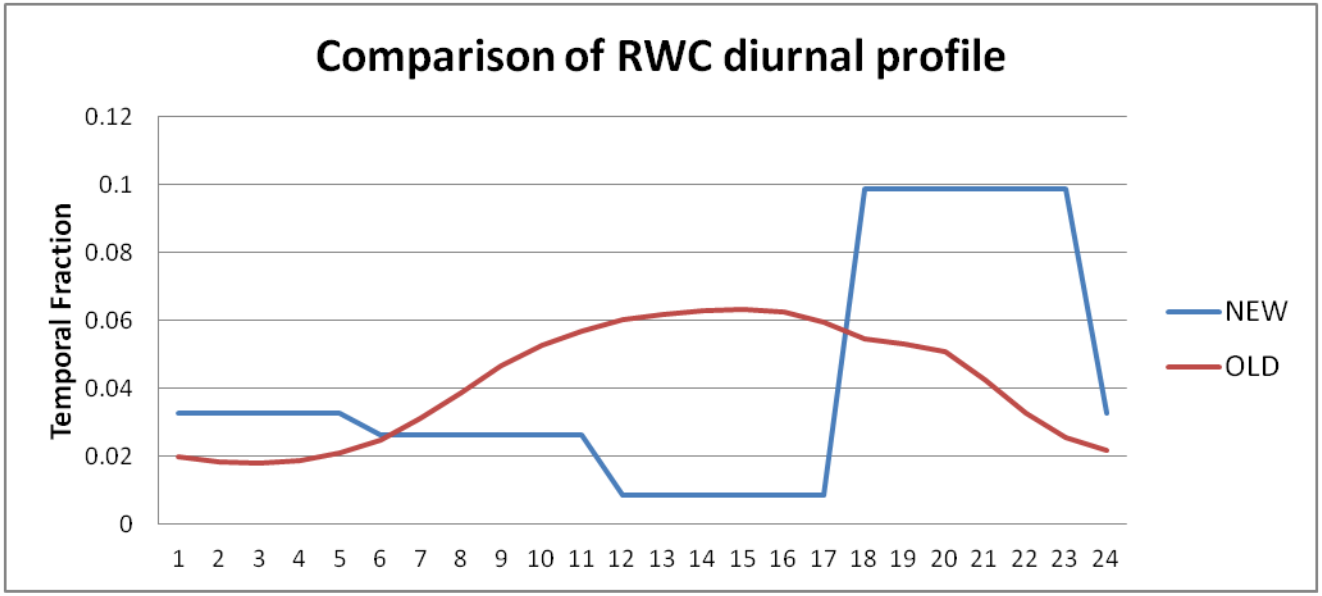
- Temporal allocation is the process of allocating inventory emissions to hourly emissions
- Hierarchy of temporal allocation steps: annual -> month -> day -> hour
- There are many types of temporal profiles for each resolution and each has a unique code
  - Typically, SCCs are used to map temporal profiles 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

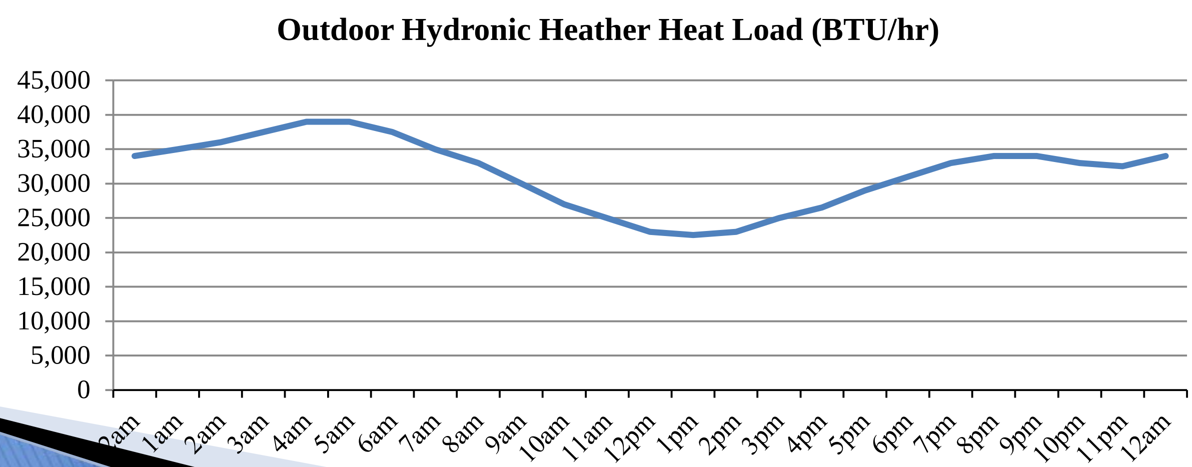
Temporal Profile Examples (1/2)





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

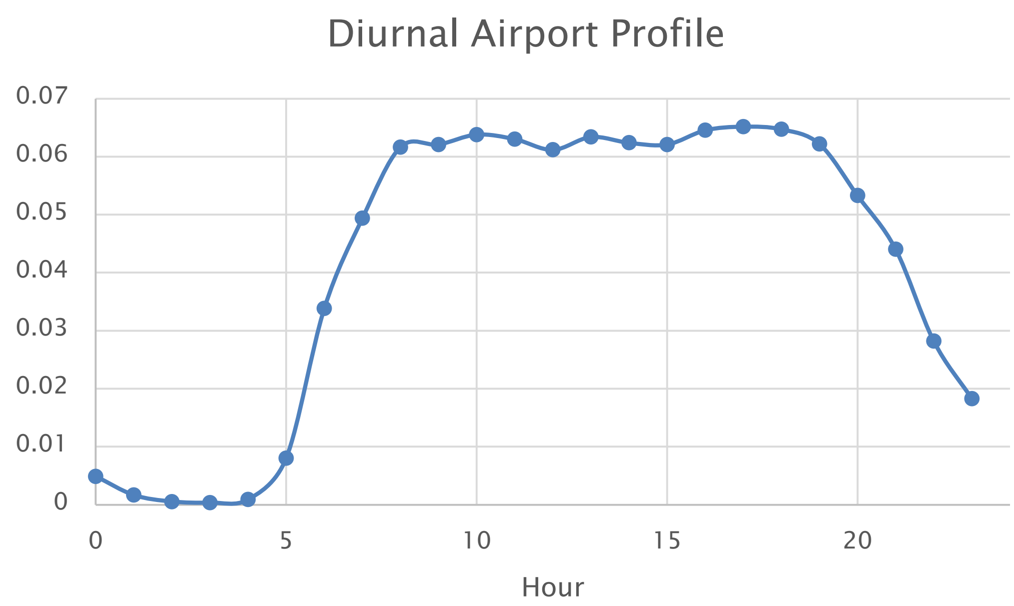
Platform sector short name	Inventory resolutions	Monthly profiles used?	Daily temporal approach	Merge processing approach	Process Holidays as separate days
afdust_adj	Annual	Yes	week	all	Yes
ag	Annual and Daily	Yes	all, hourly met	all	Yes
agfire	Annual	Yes	mwdss	mwdss	Yes
ptagfire	Daily	No	all	all	Yes
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

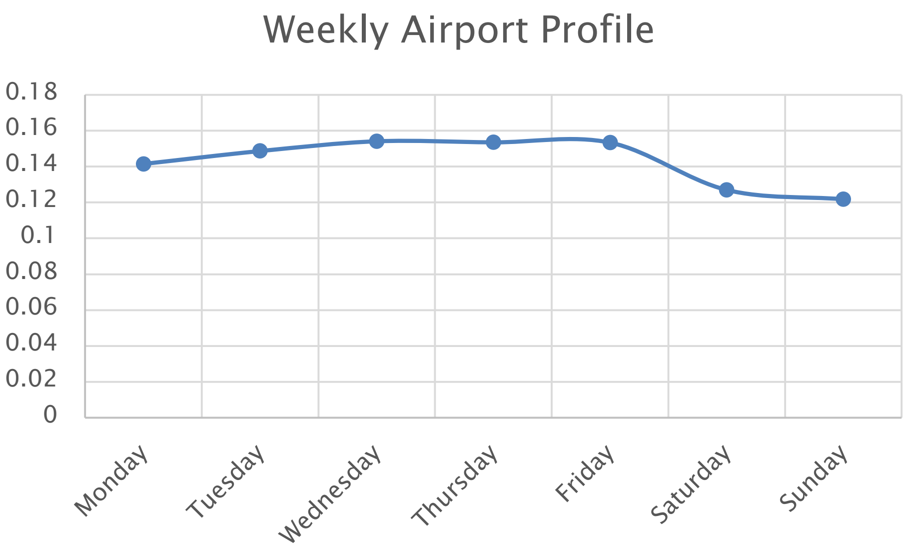
Airport Temporalization (1/2)

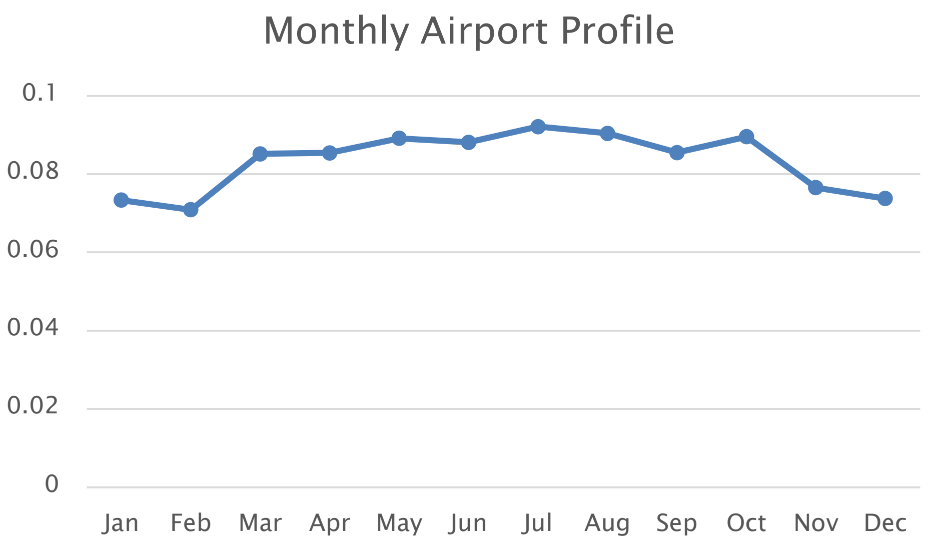
- Airport diurnal temporal profiles updated for 2014v7.0 platform based on Aviation System Performance Metrics (ASPM) Airport Analysis
  - https://aspm.faa.gov/apm/sys/AnalysisAP.asp



Airport Temporalization (2/2)

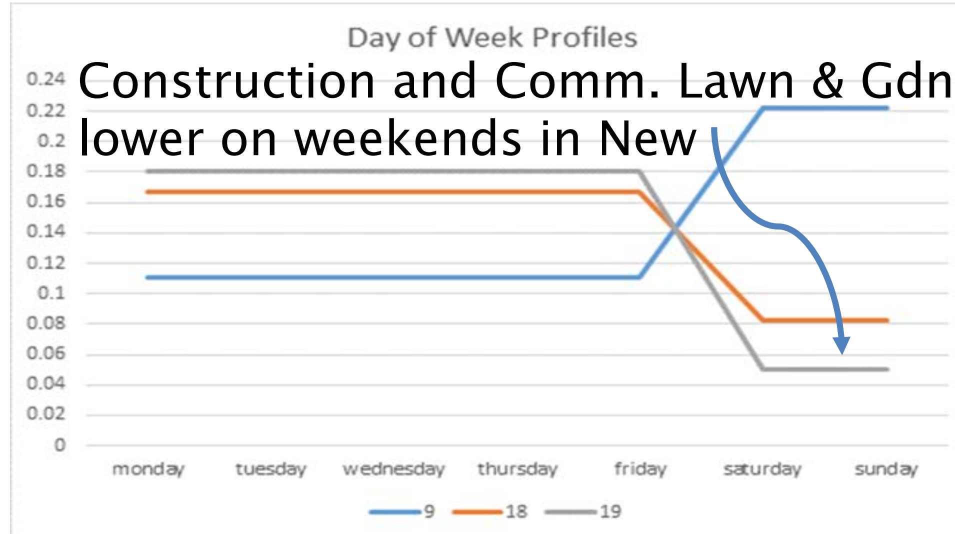
- Weekly and monthly profiles based on FAA Operations Network Air Traffic Activity System
  - http://aspm.faa.gov/opsnet/sys/Terminal.asp

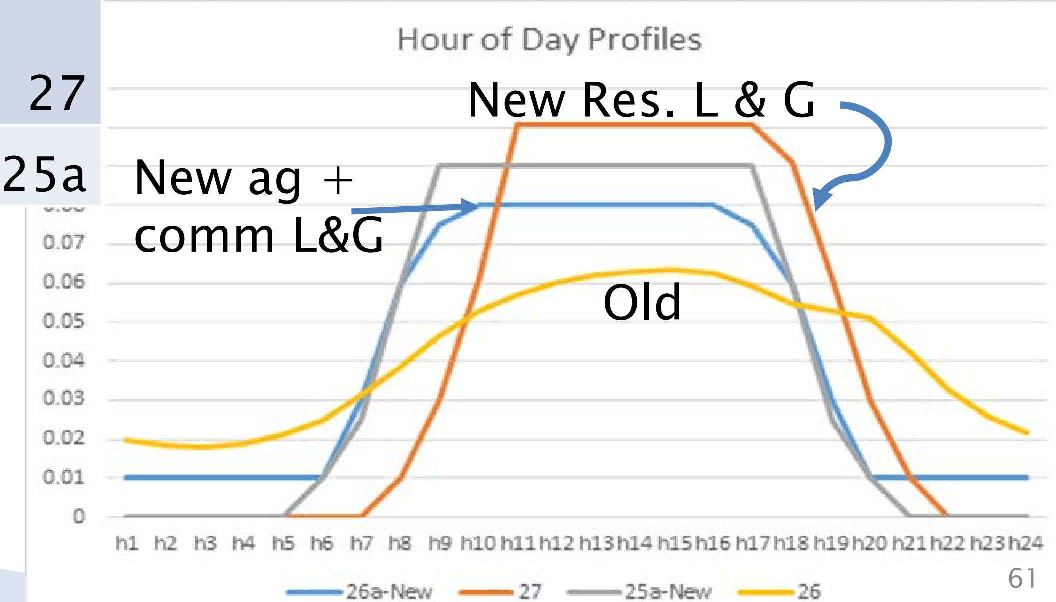




Nonroad Temporal Profile Updates

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





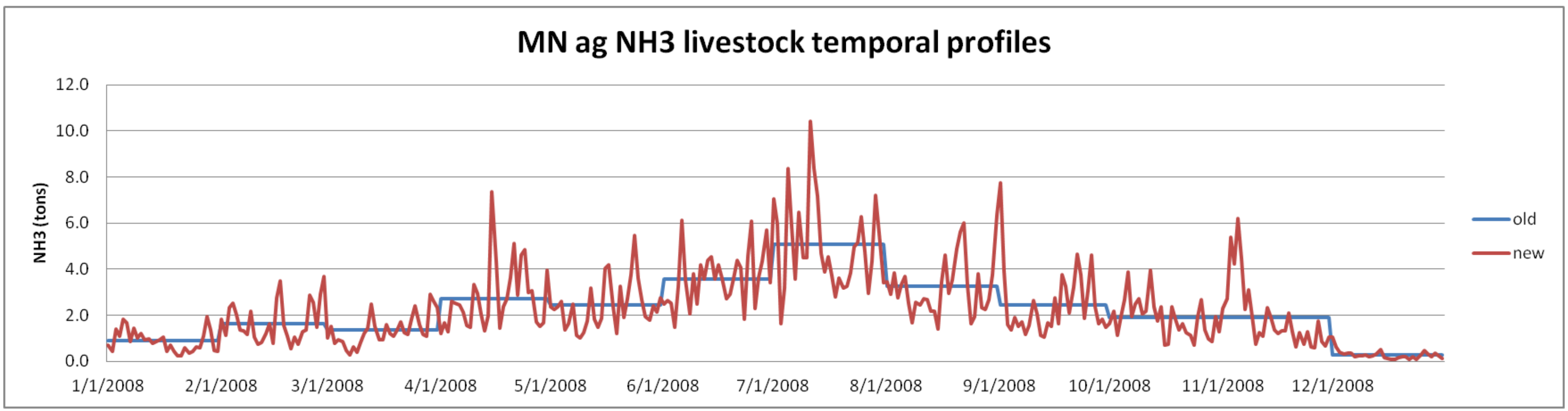
New diurnal profiles have lower overnight emissions

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)

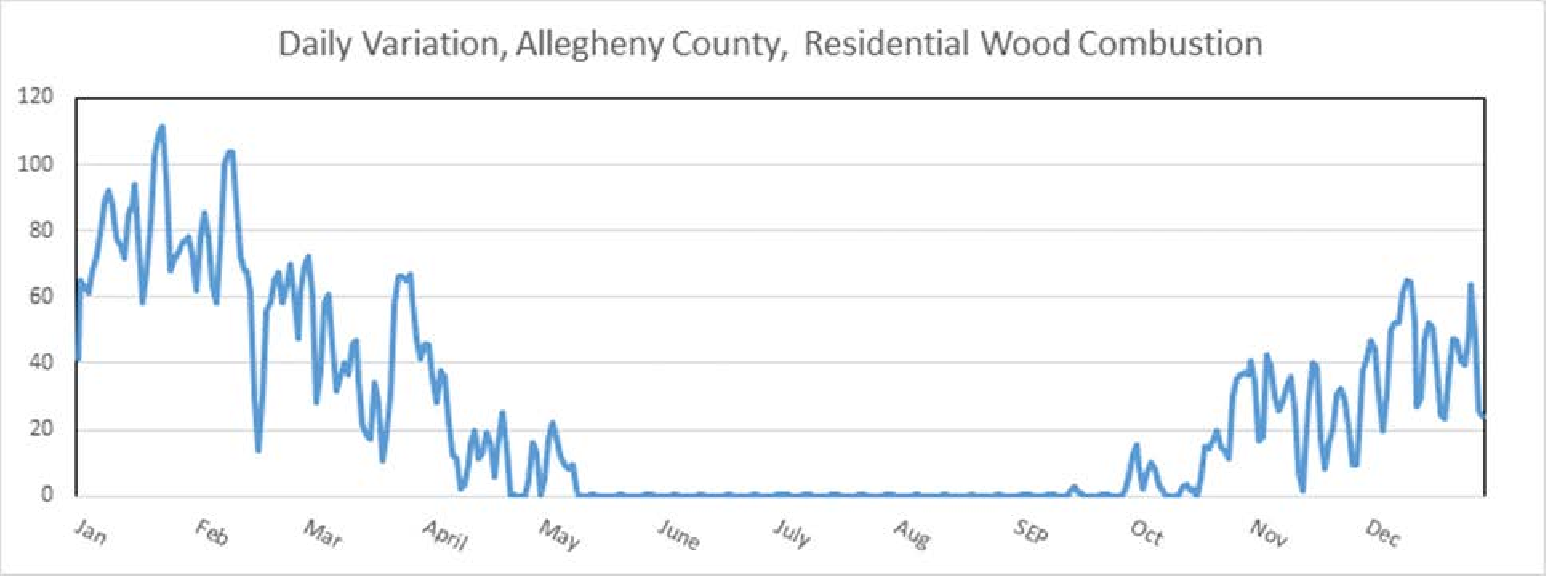
GenTpro: ag livestock

- 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



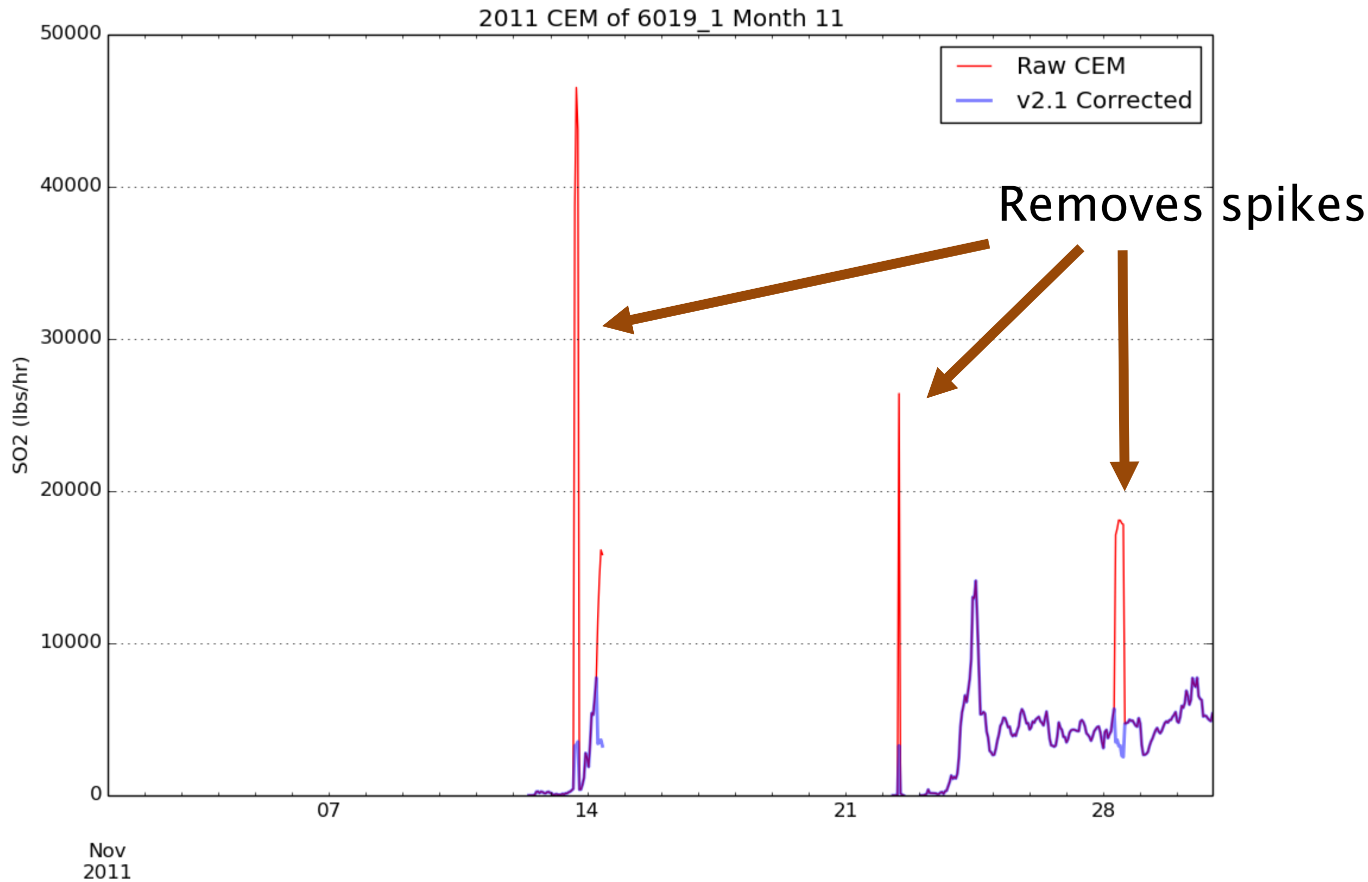
Special Steps for EGU Temporalization

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 any 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

EGU Temporal Profiles and Matching

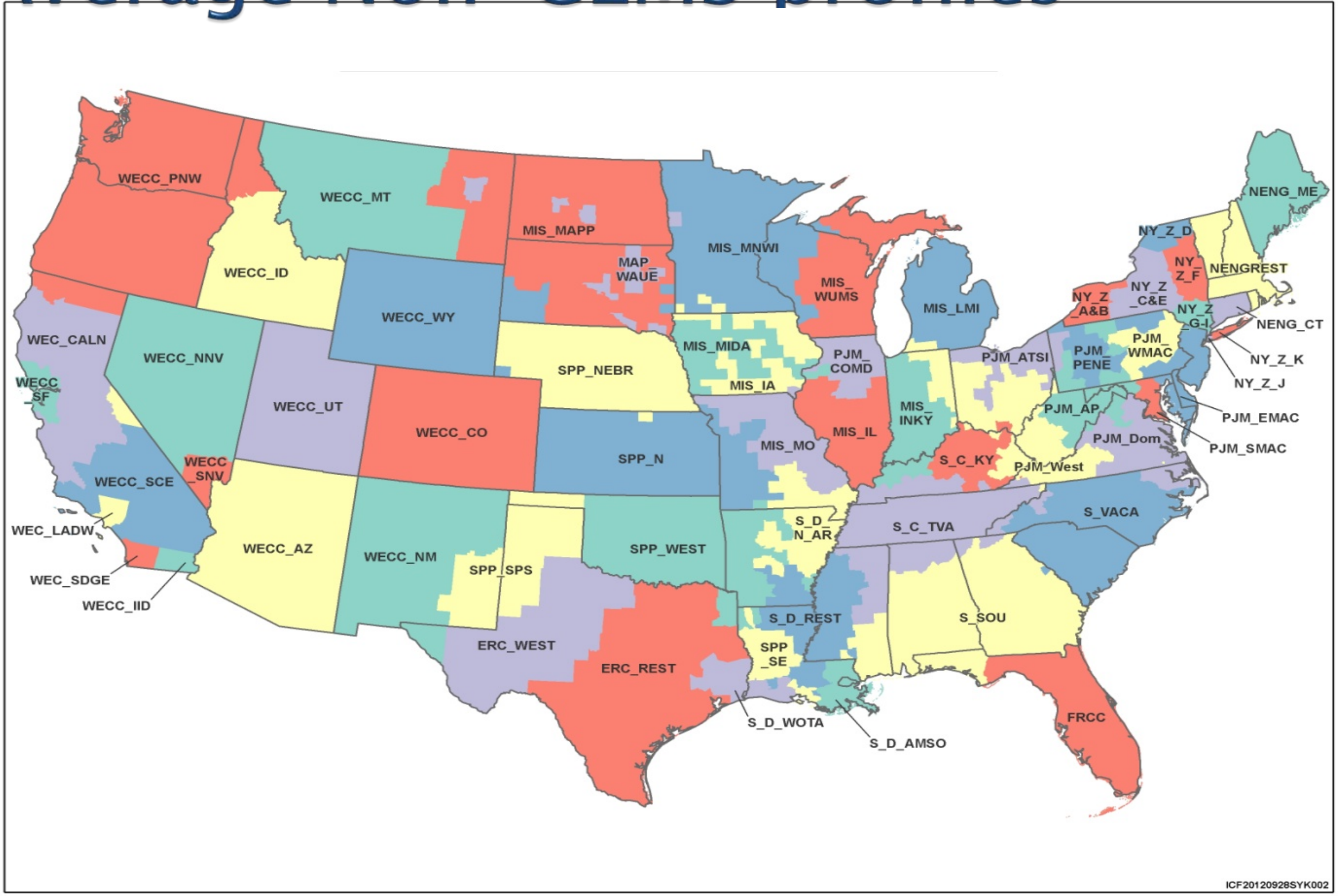
- Removed non-measured data values from CEMS data to ignore emission spikes
- Hierarchy of CEMS assignments:
  1. Use CEMS for all months (units with complete CEMS data) <-- **Note: CEMS data replace the annual NEI data**
  2. Use CEMS for months where have measurements, use regional averages for period 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

CEMS Data are run through UNC's CEMS Correction Tool



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

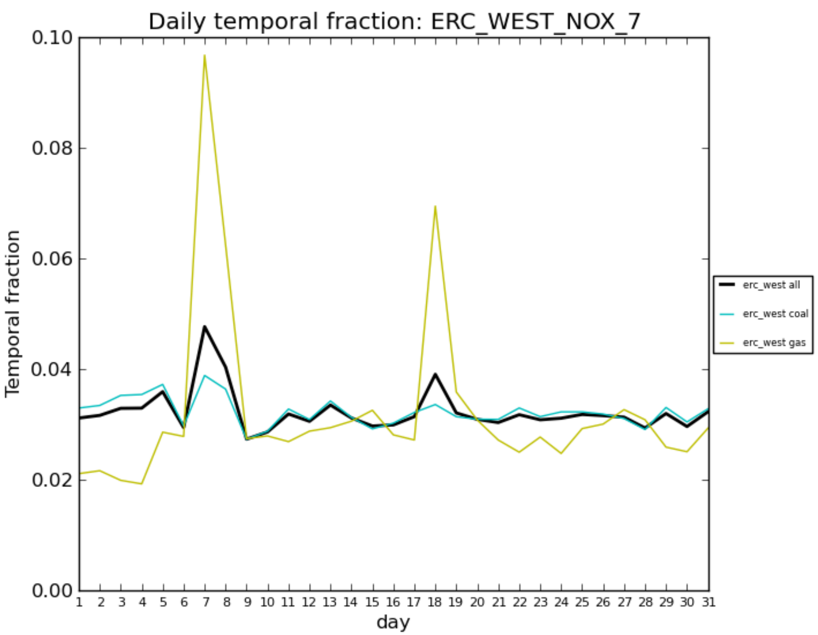
Map of IPM Regions used for Average Non-CEMS profiles



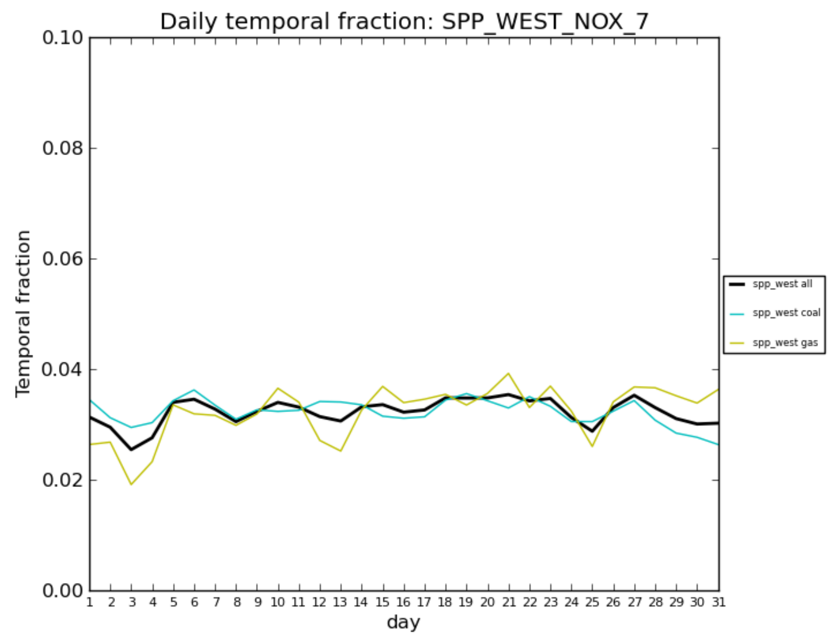
Average Month-day Profiles: Region- and fuel-specific

Profiles differ between regions

(yellow=gas, blue=coal, black=composite)

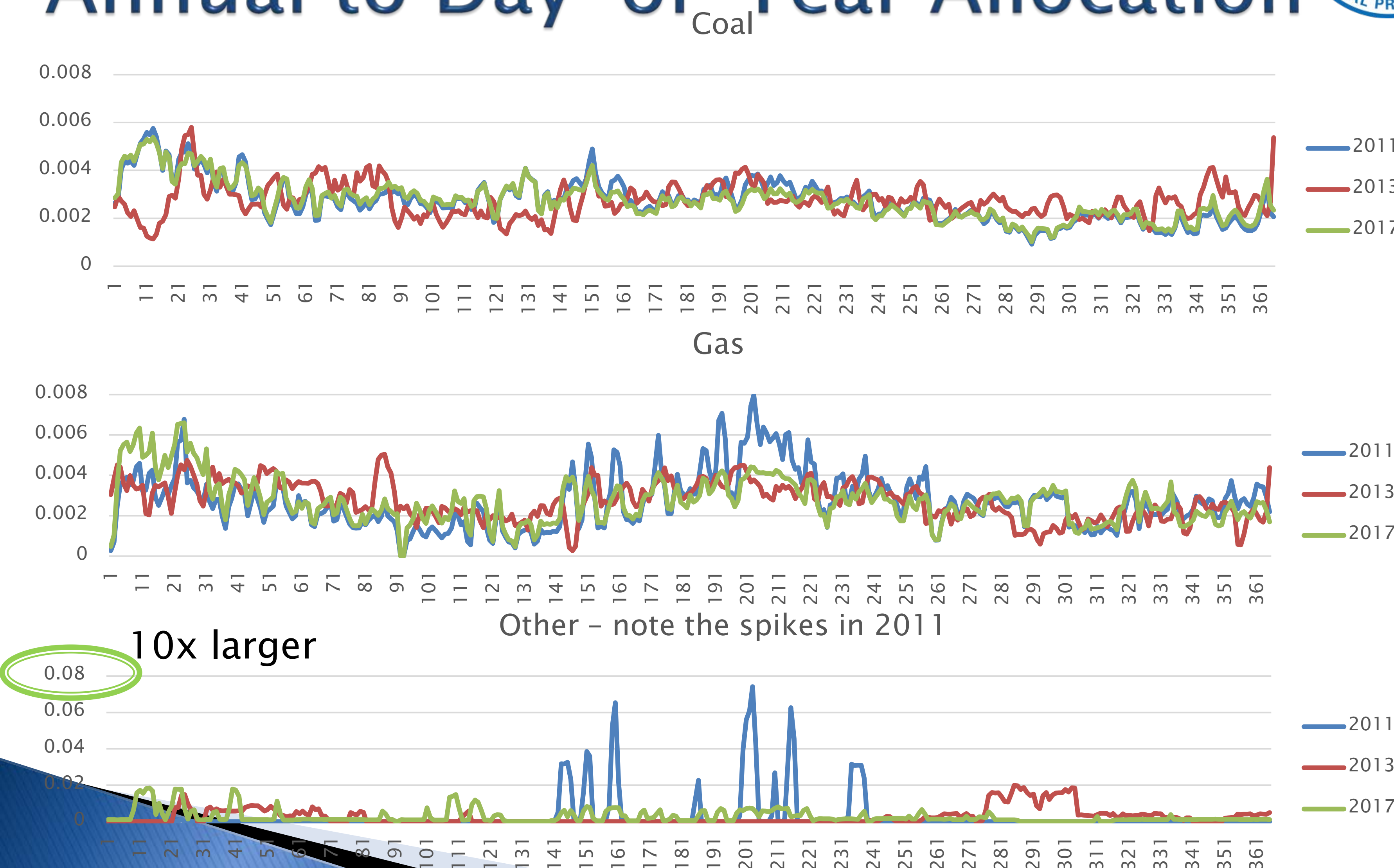


IPM Region in W Texas

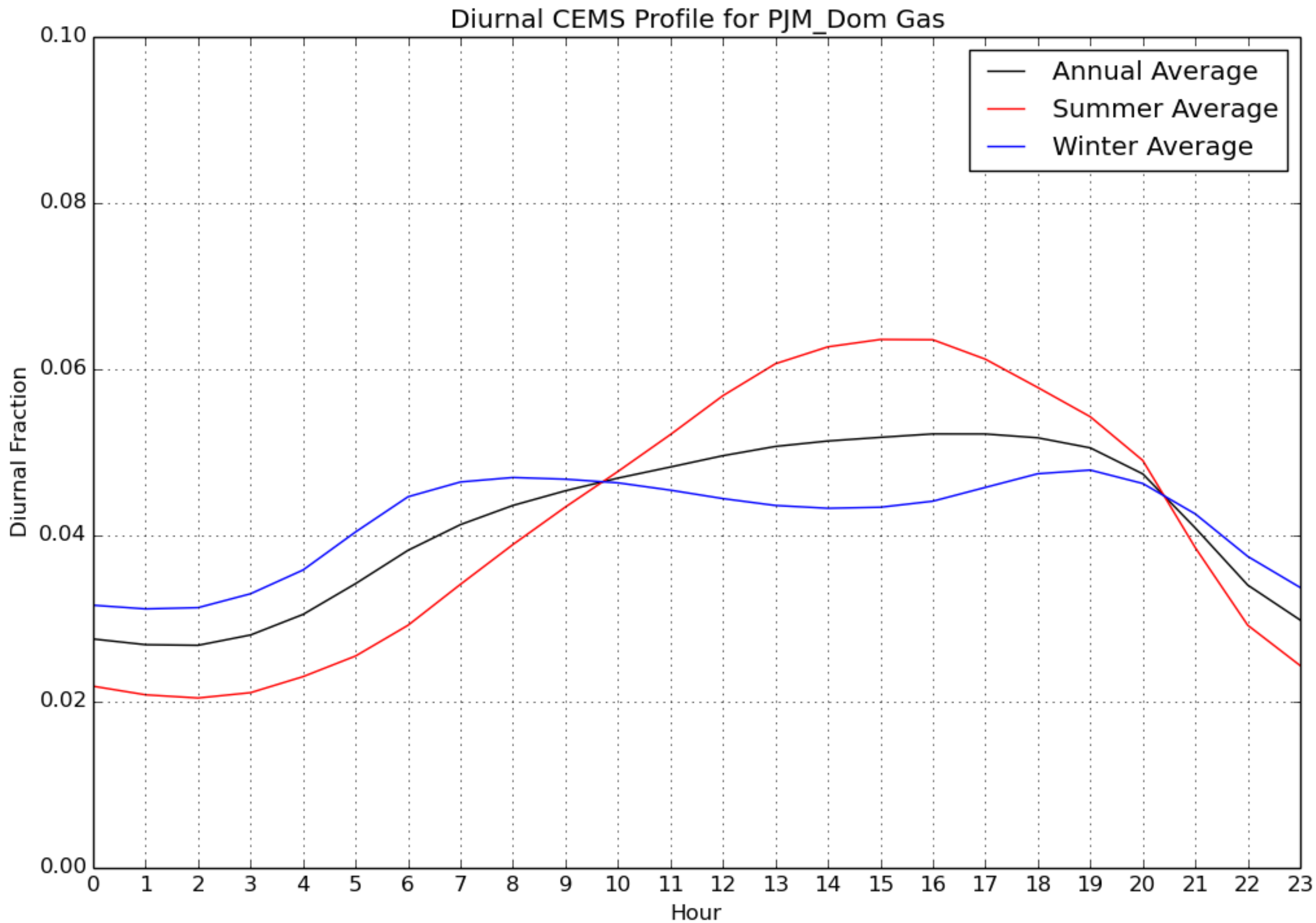


IPM Region in E Oklahoma and W Arkansas

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

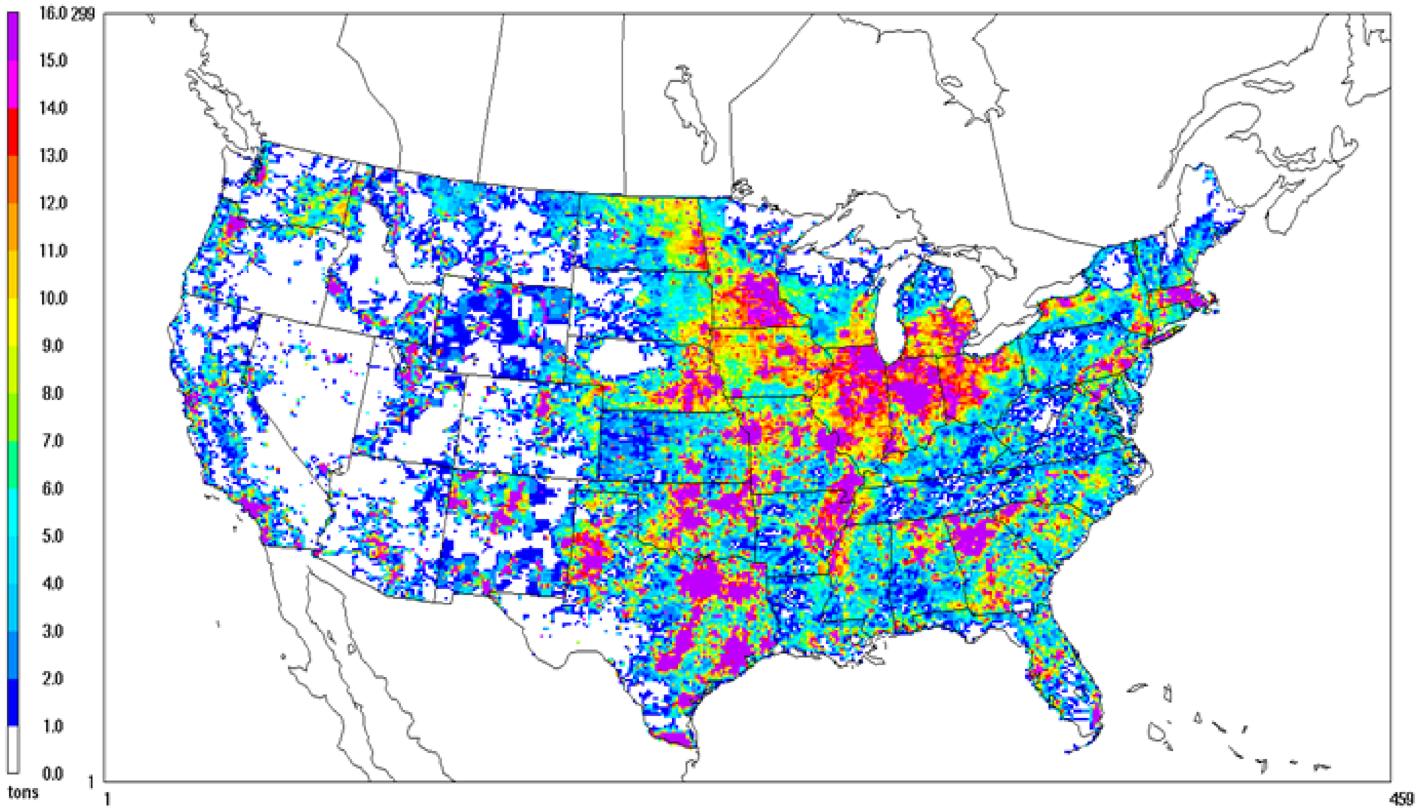
- Check SMOKE temporal logs to ensure all sources have reference to temporal profiles
- Sum post-SMOKE daily emissions by sector to compare back to annual for inventory comparison
- Perform various specialized analysis of EGUs (partial year reporters, spikes in CEMs data)
- Check the PTSUP files to confirm 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

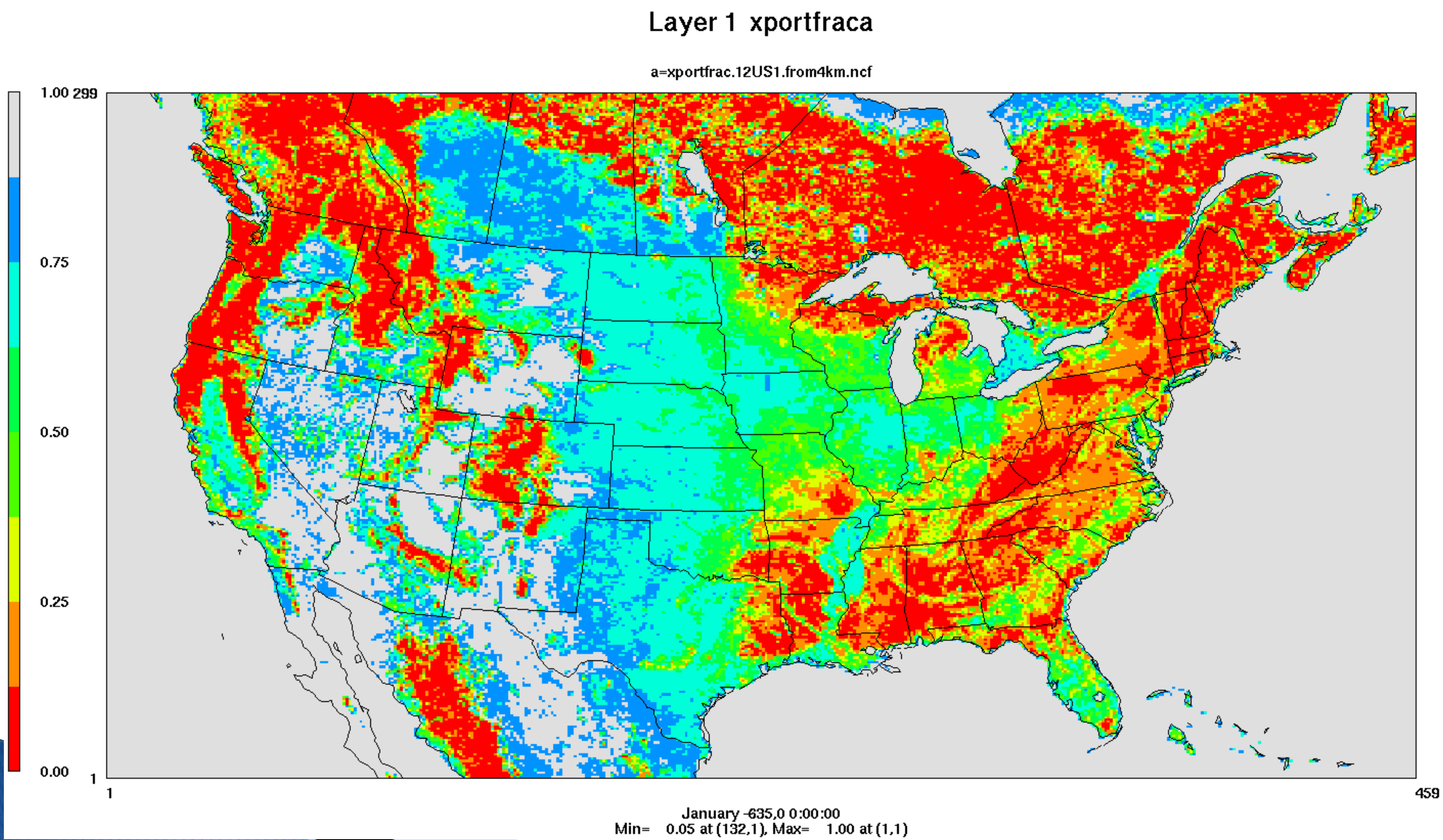


Afdust Adjustments: Transport Fraction

- 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

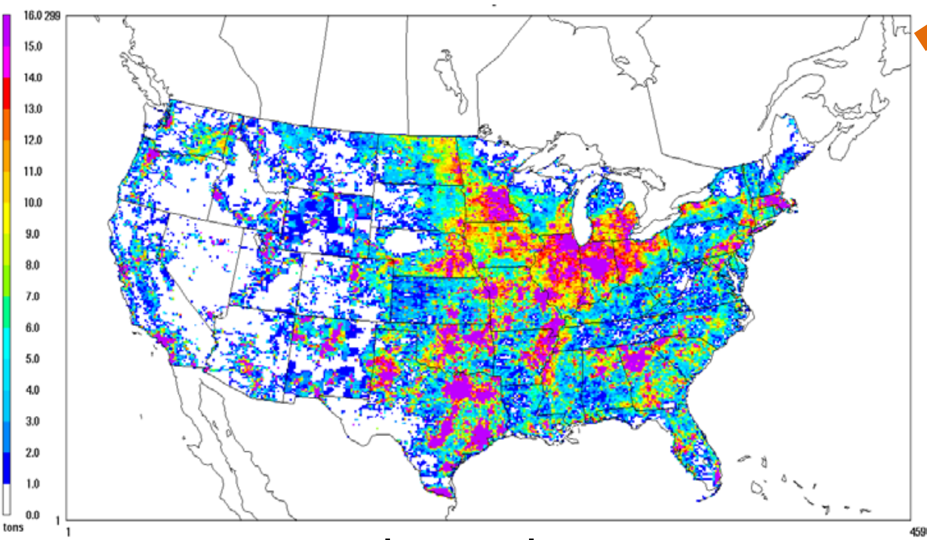
Transport Fraction Plot

Red = high level of reduction; Gray = little reduction



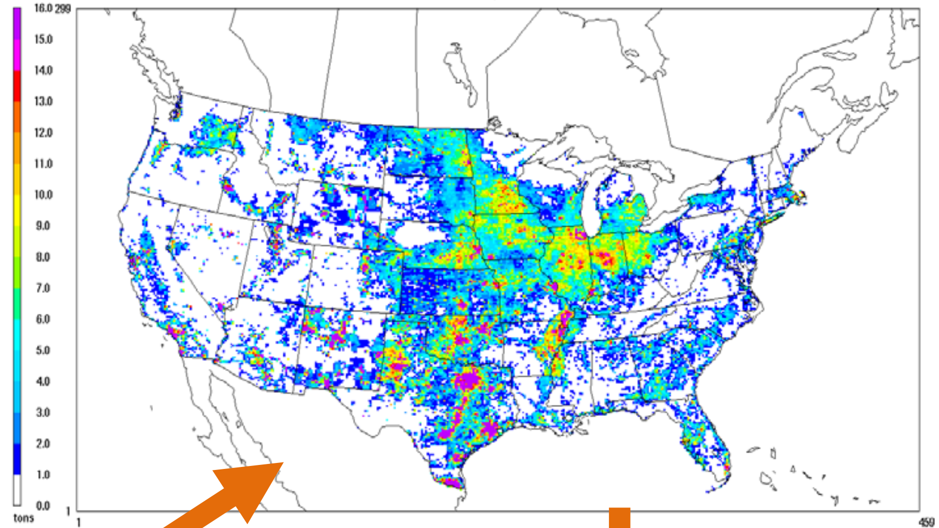
Impact of afdust Adjustments

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

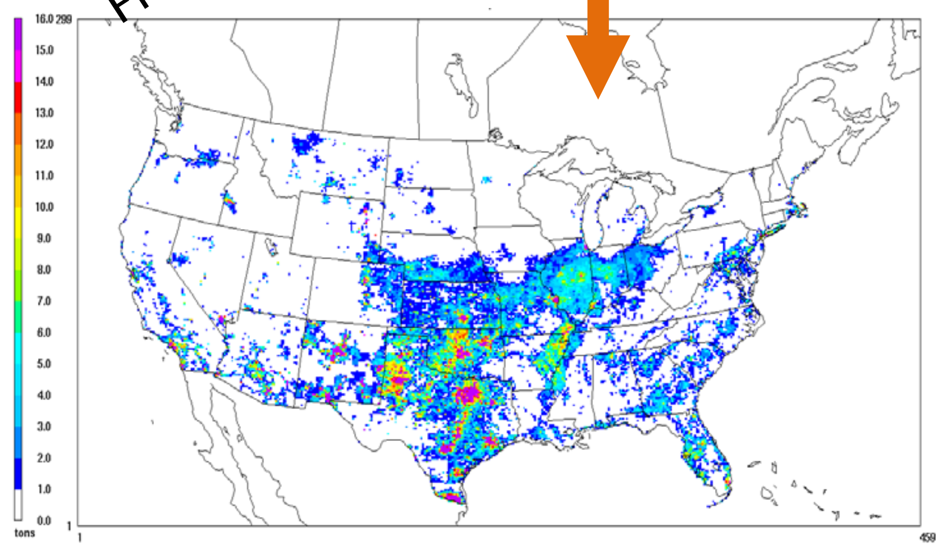


Unadjusted emissions

Apply Transport Fraction



Apply 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

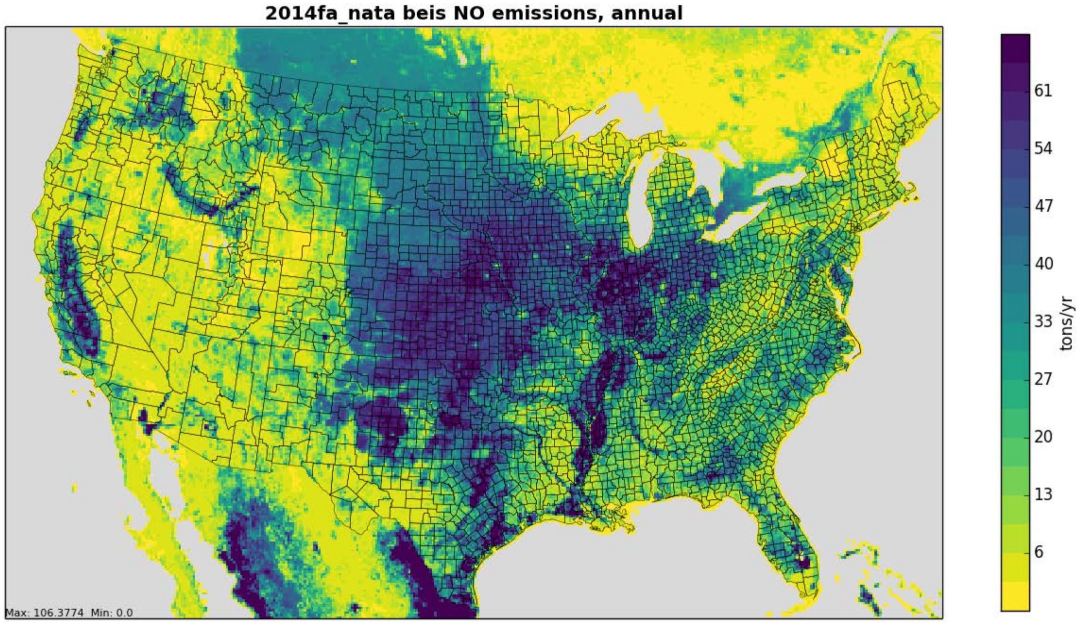
Meteorological Variables Needed for BEIS 3.61

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

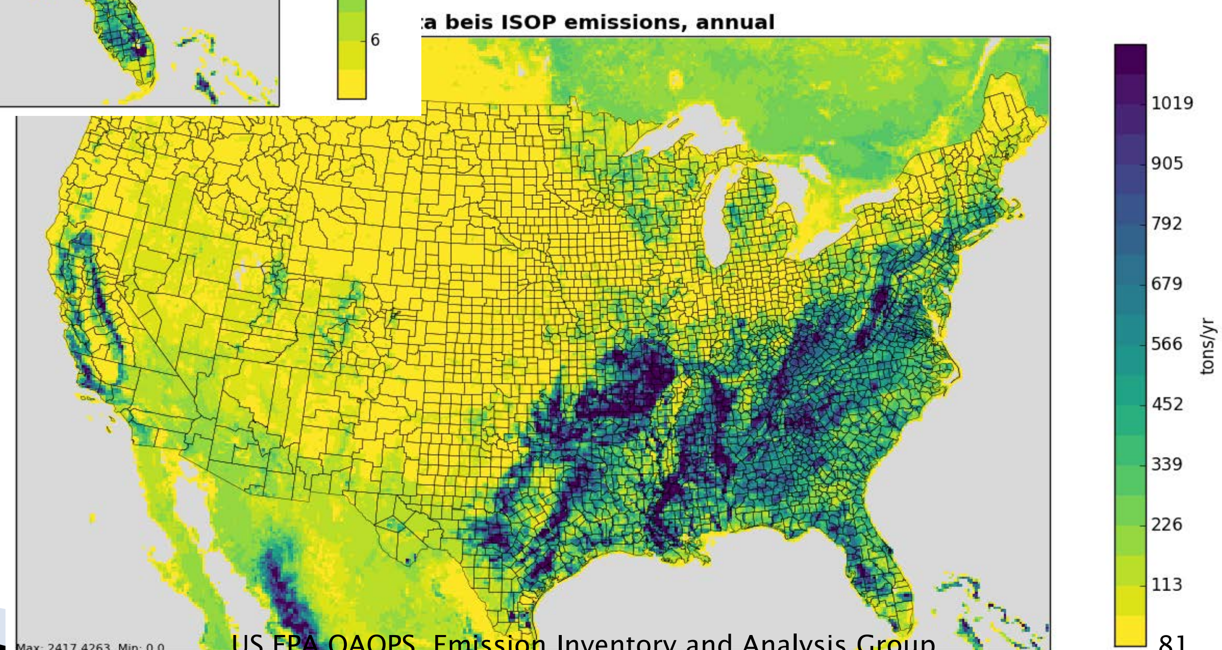
Species Produced by BEIS

- 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?

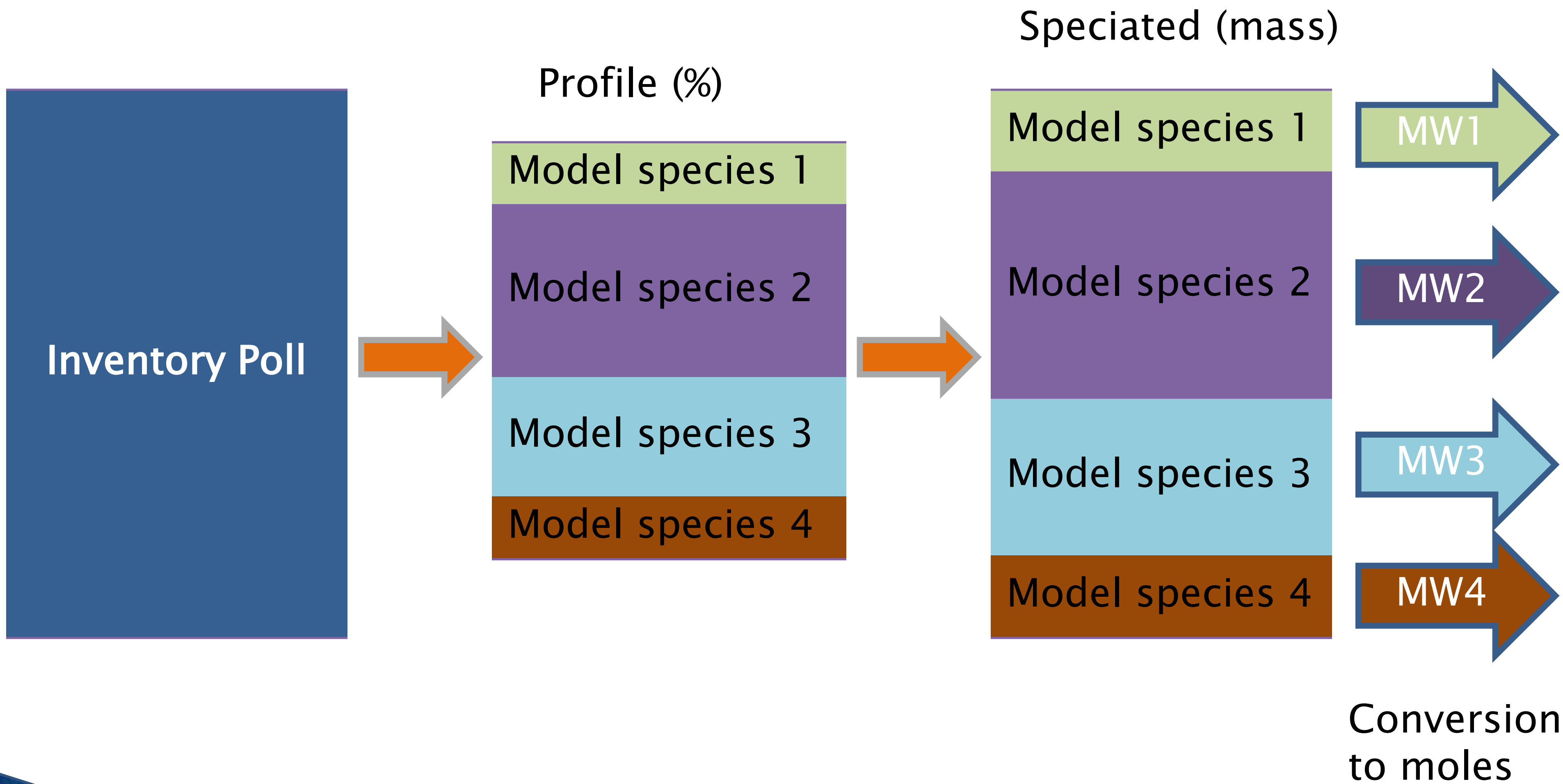
Speciation

- 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

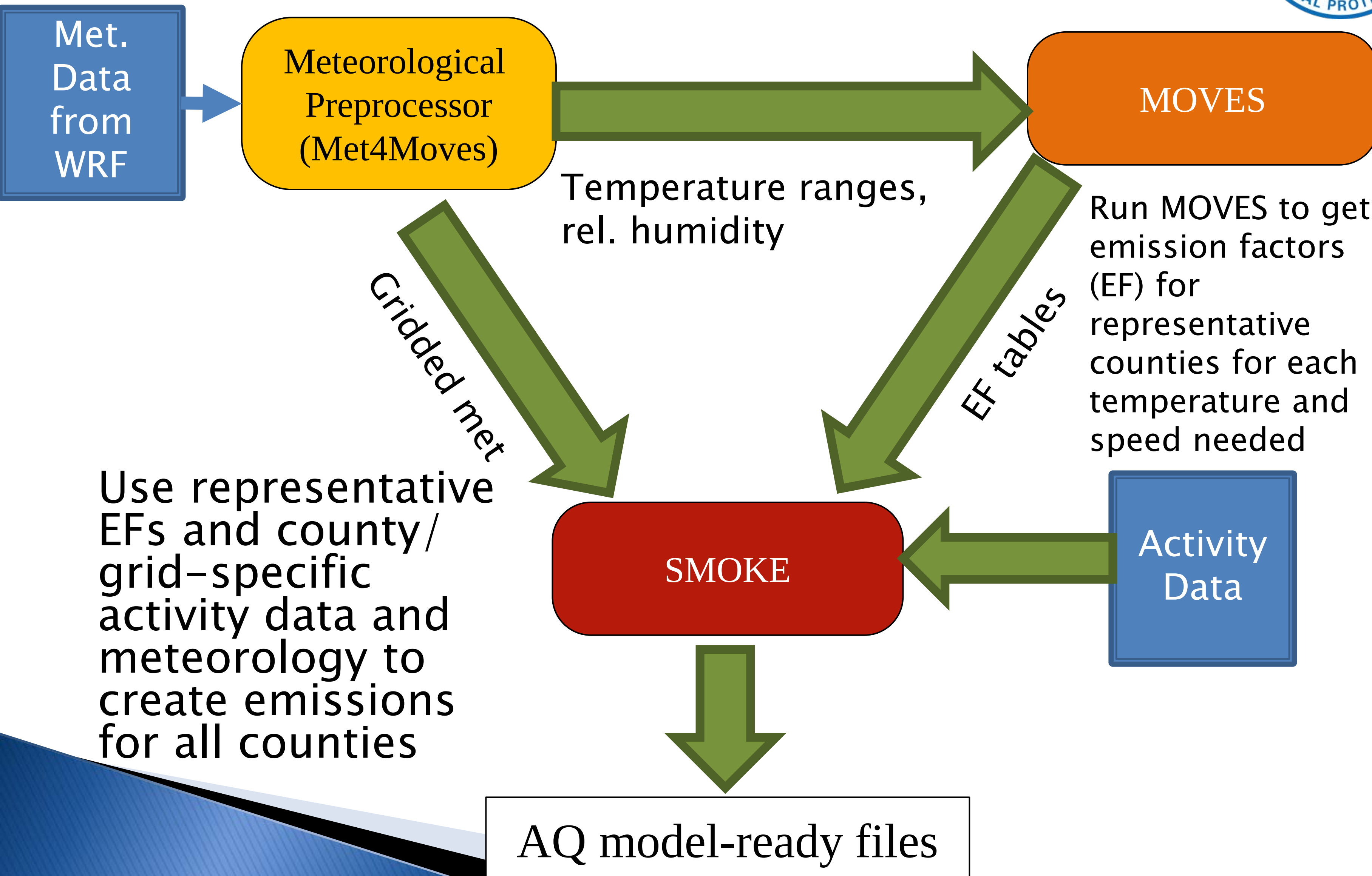
QA of Speciation

- 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?

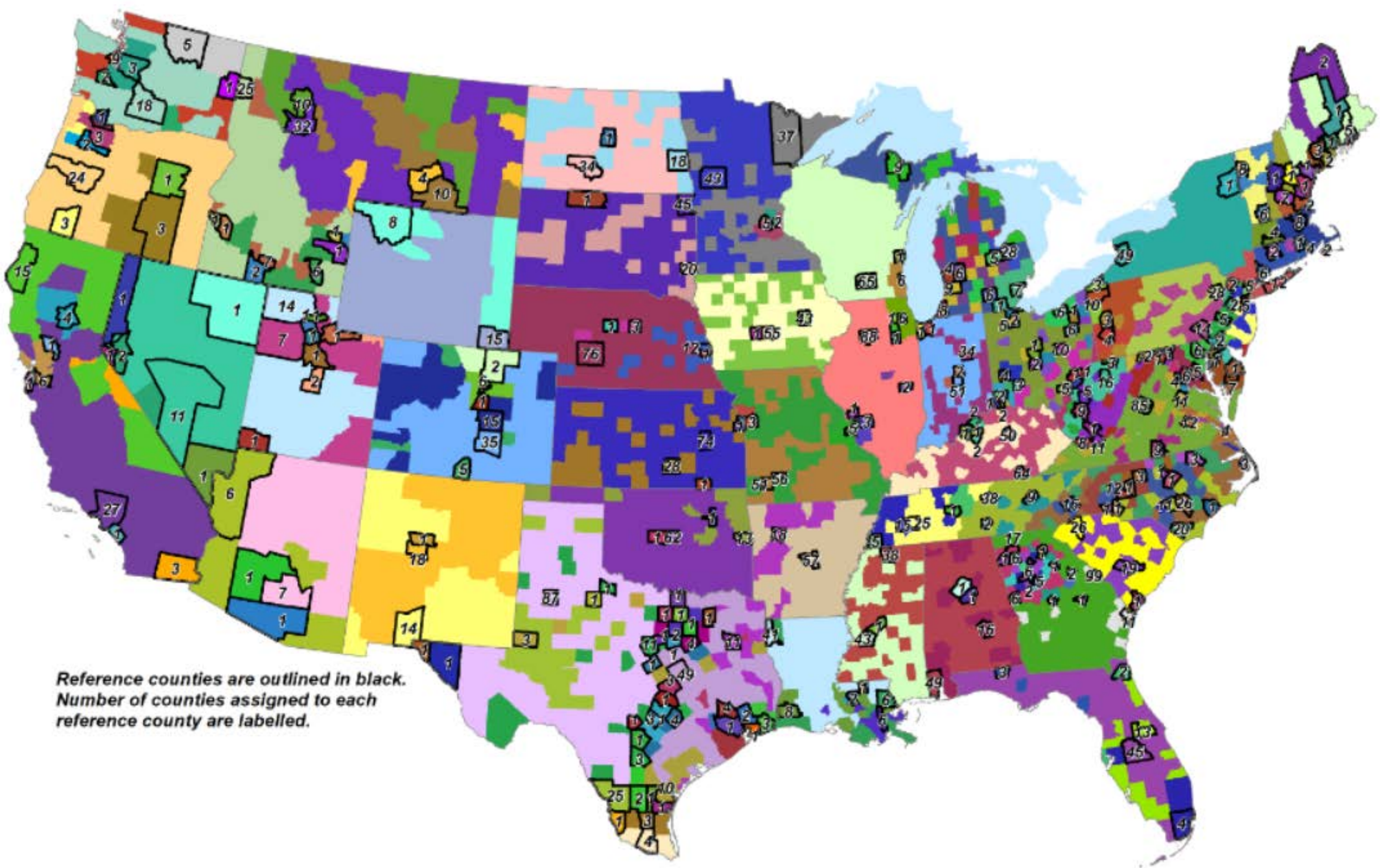
- Any questions on speciation?
- There is a training class on Speciation tomorrow
  - If you haven't signed up, there will be slides that you can download after the conference

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

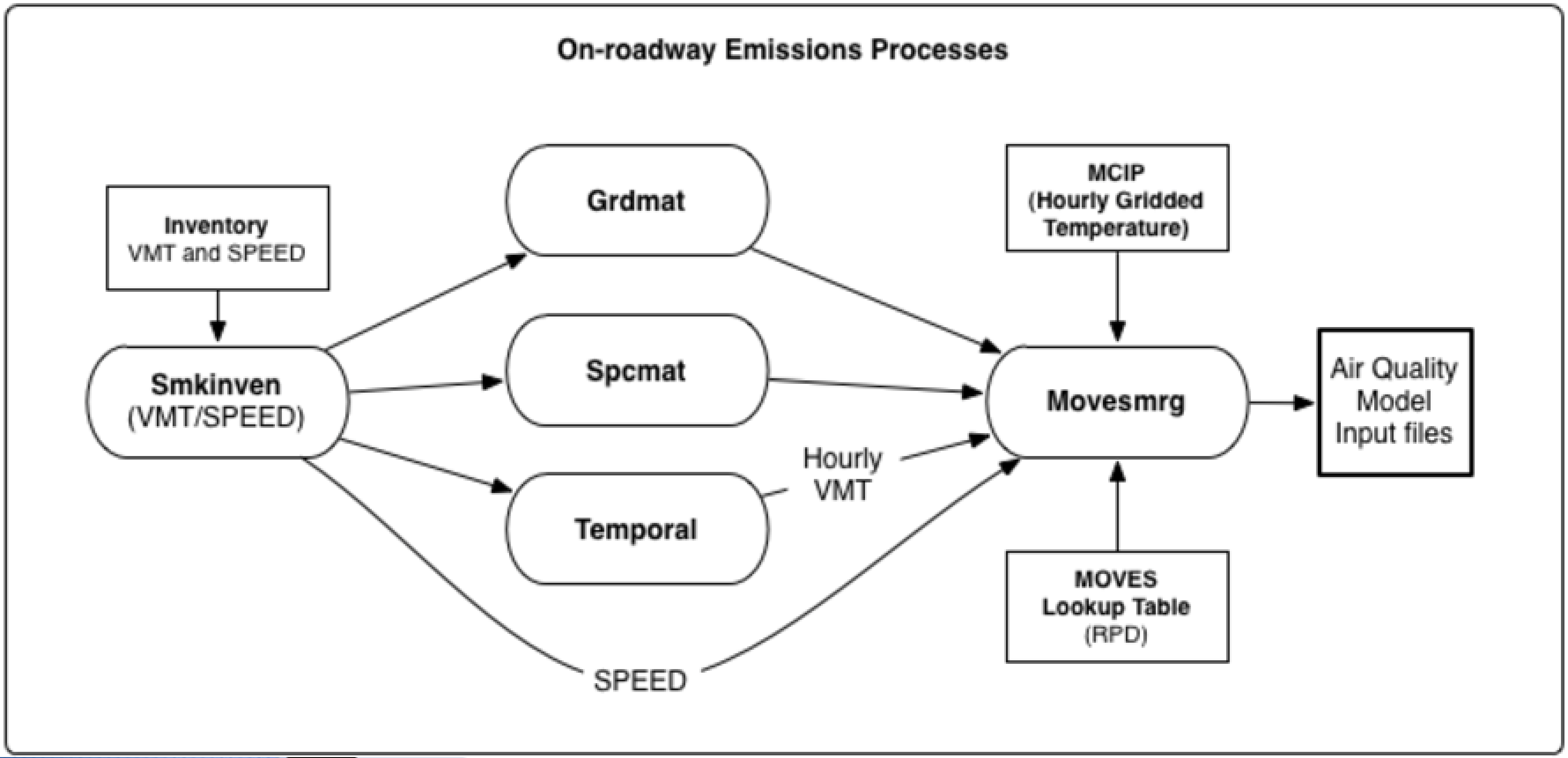


Emission Processes in SMOKE/MOVES

- 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 emissions (i.e. from 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)

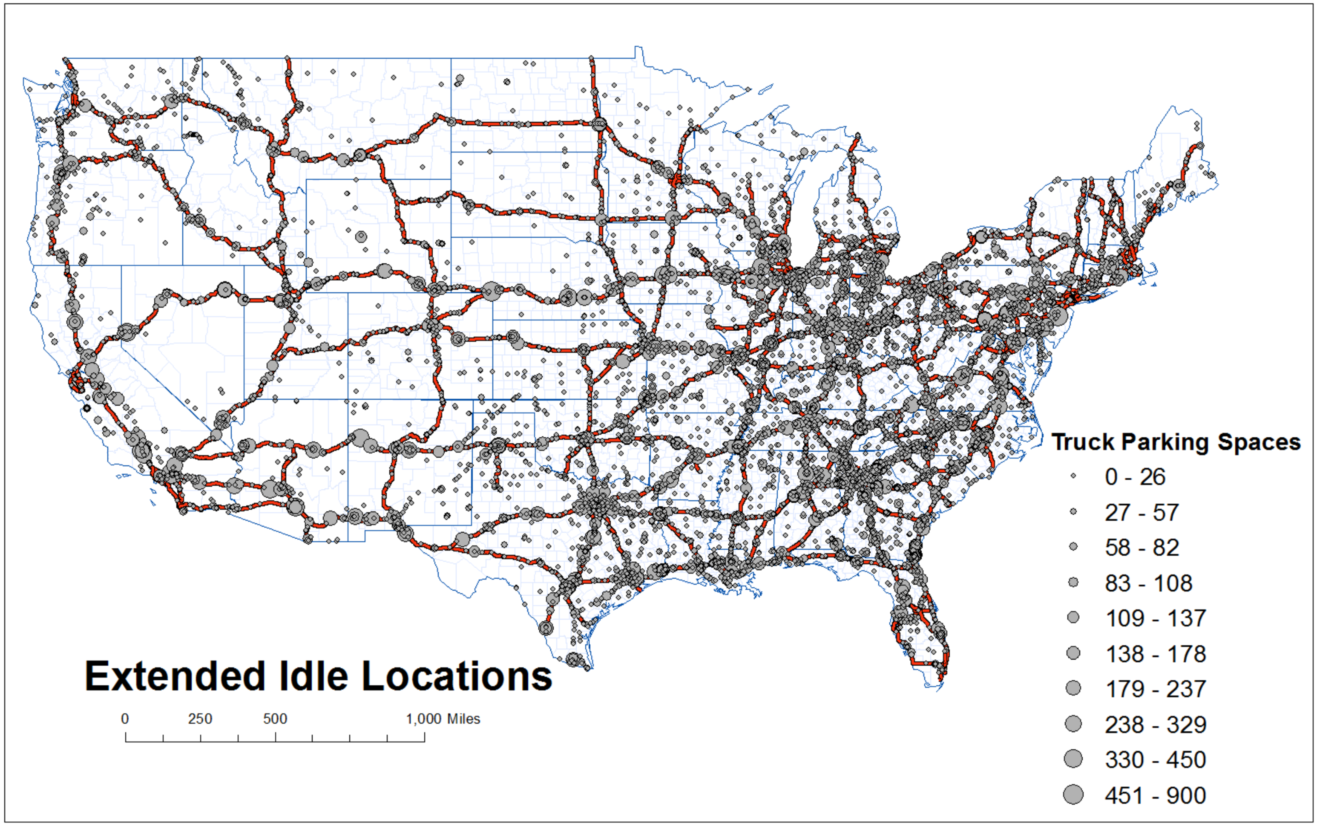
On-roadway Processing (RPD)

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



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



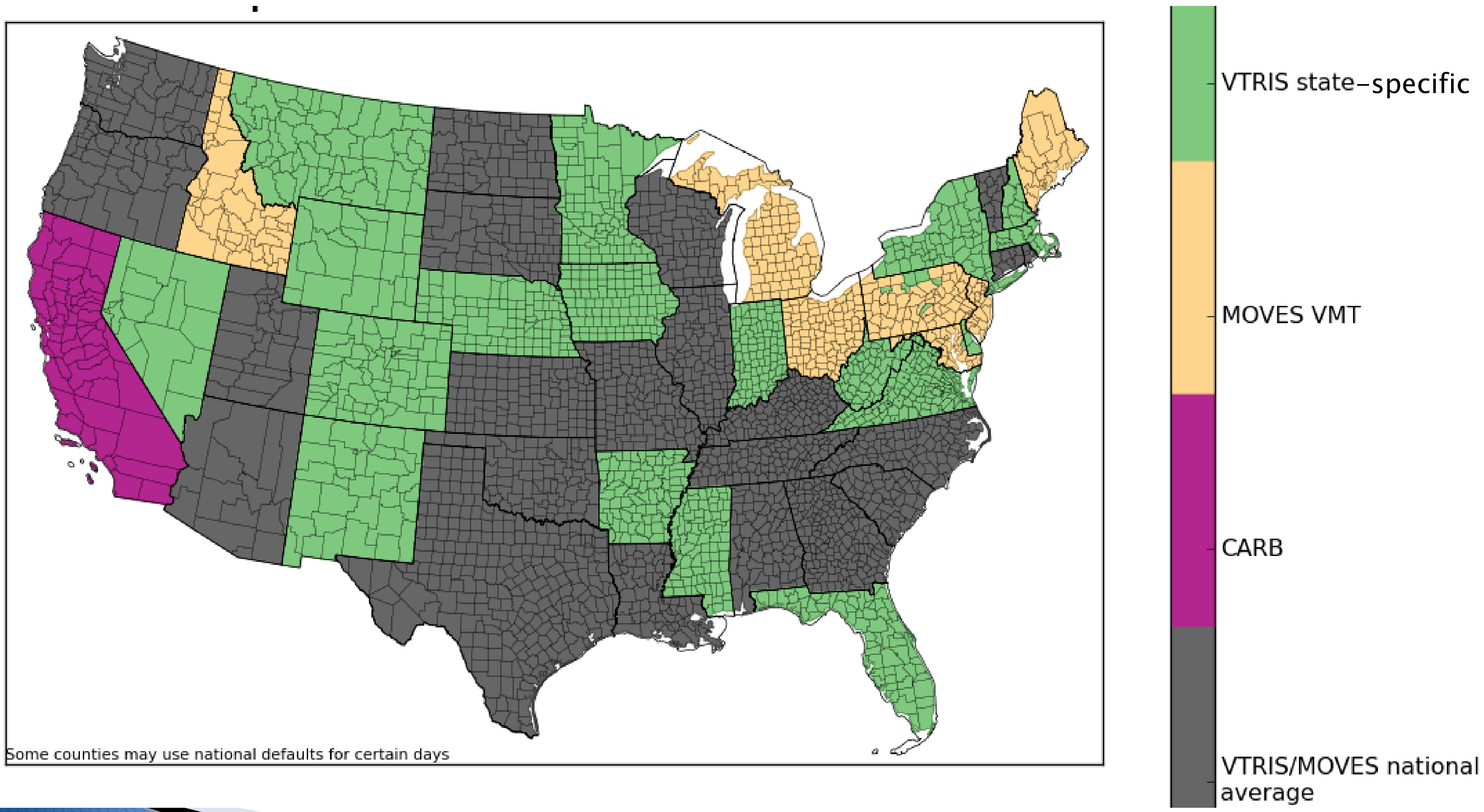
Recent Onroad Emissions Modeling Developments

- 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

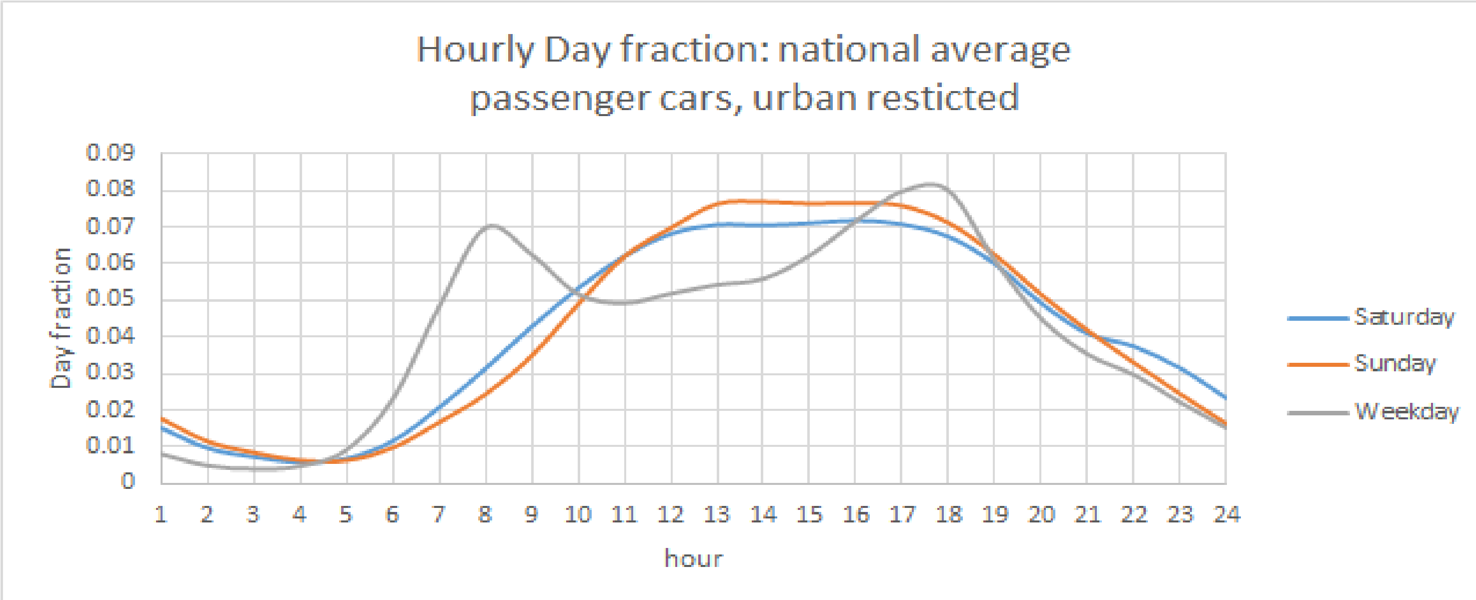
Onroad Temporal Profiles

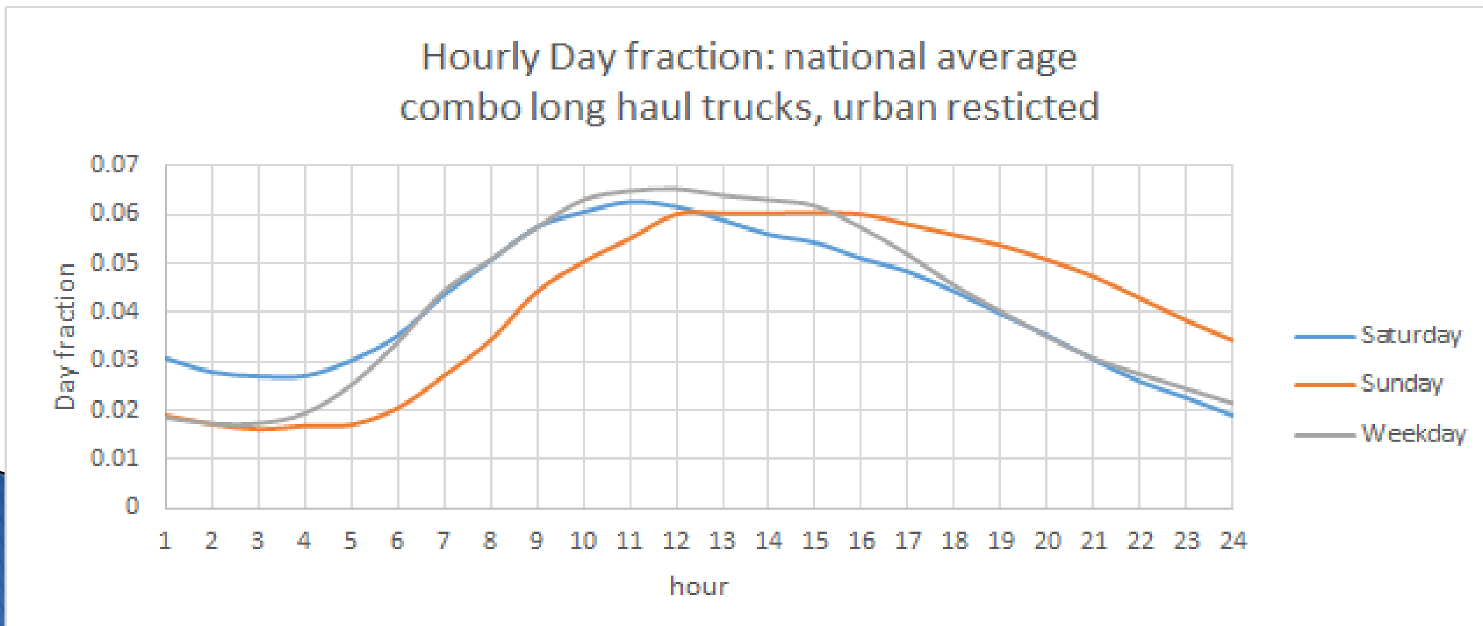
- Temporal profiles based on 2012 Vehicle Travel Information System (VTRIS) data
  - Reported traffic count data to the Federal Highway Administration (FHWA)
  - Varies by state , HPMS vehicle (10, 20, 30, …) and road type
  - Distinct hourly / diurnal profiles for weekdays/Sat/Sunday
  - Day of the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

Temporal Profile Data Sources



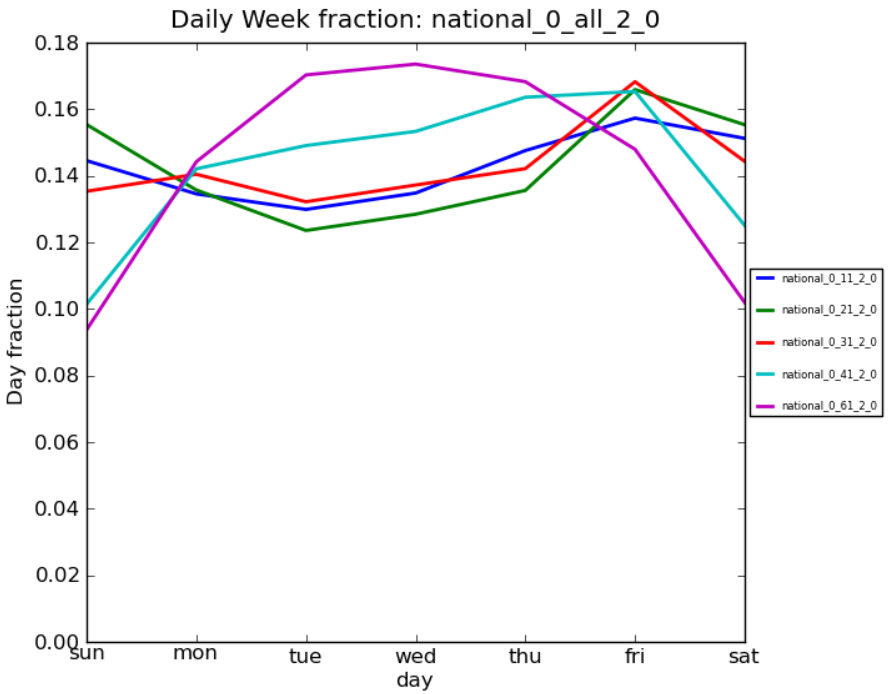
National Default Diurnal Temporal Profiles

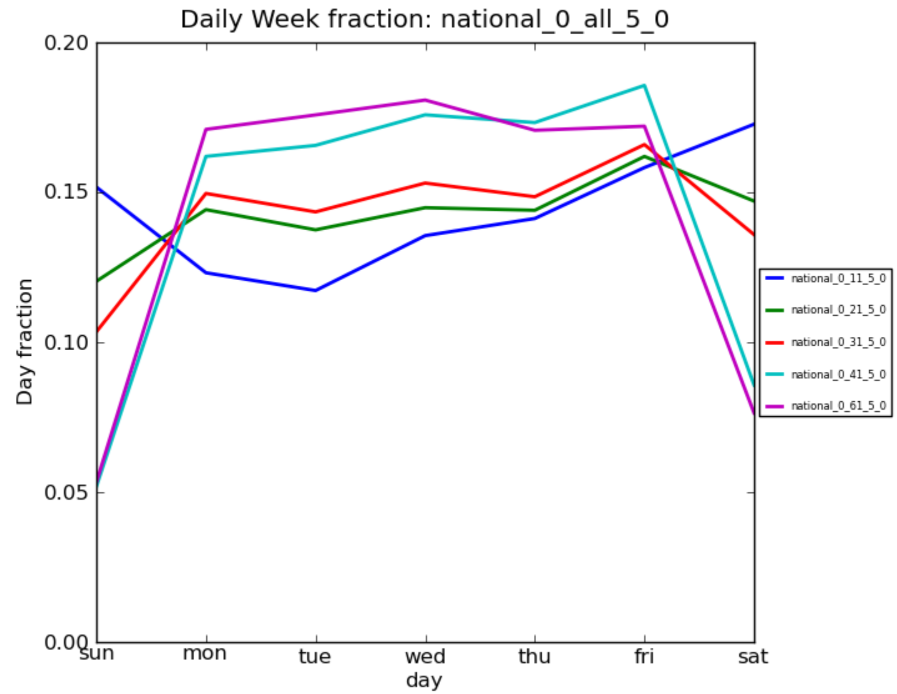




National Day of Week Temporal Profiles

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

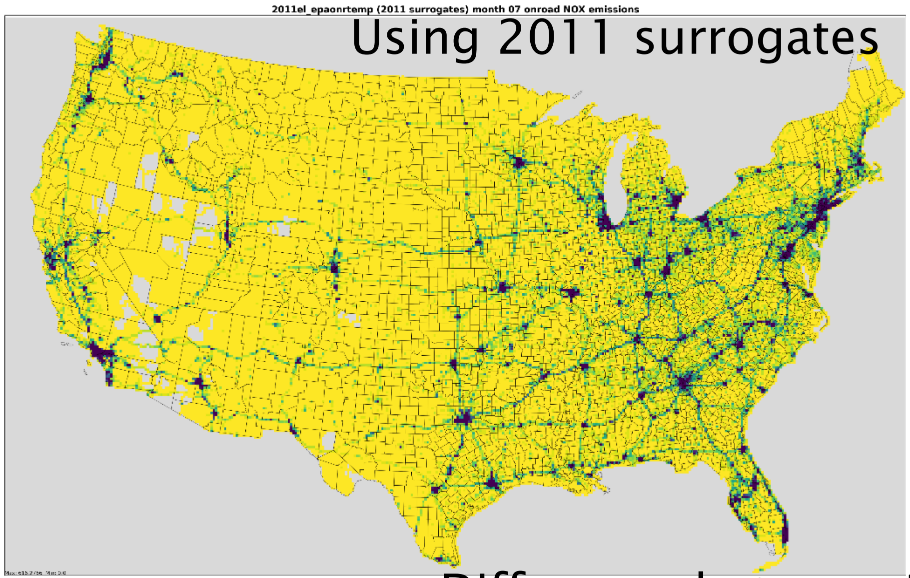


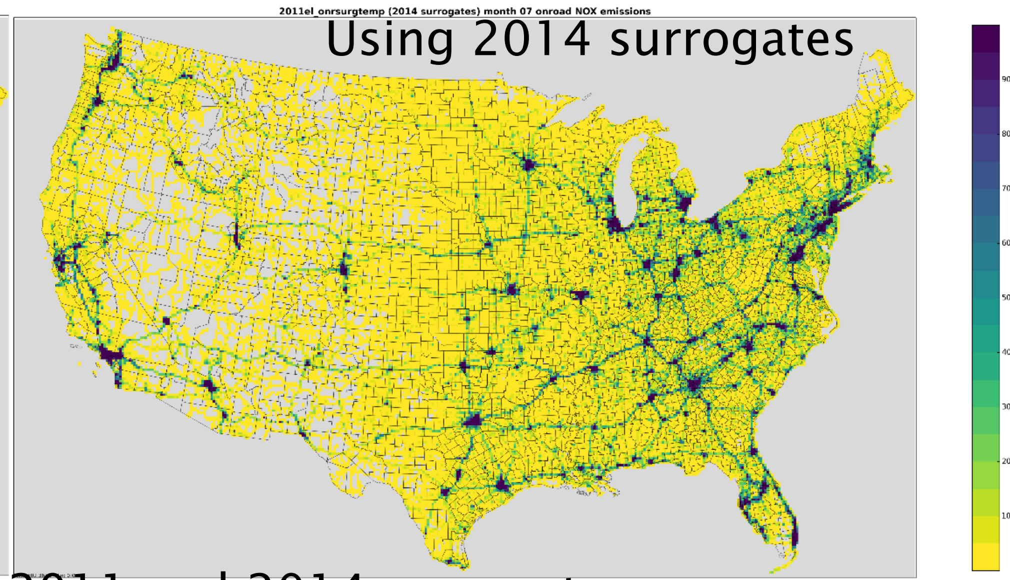


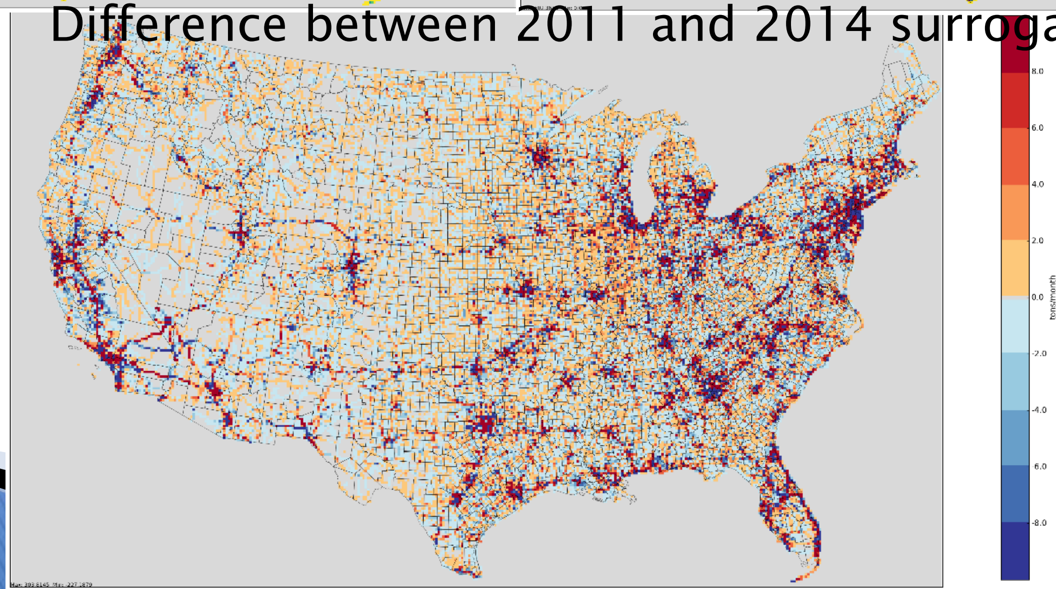
Rural restricted:
light-duty have Friday peak

Urban unrestricted:
more traffic weekdays

Impacts of new Spatial Surrogates on 2011 Onroad NOx Emissions







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 – approximately 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
16	Indiana	1,444,822	71,636	392,145	205,392	112,103	345,897	272,213	2,487	3,788	3,774
17	Iowa	724,179	296,254	206,780	197,567	59,452	93,062	162,909	2,791	2,494	3,980
18	Kansas	936,933	206,901	283,560	453,030	115,071	43,352	278,783	4,245	3,057	8,531
19	Kentucky	1,117,918	57,483	291,863	138,749	75,395	222,175	290,896	3,673	3,709	7,697
20	Louisiana	1,888,754	79,071	369,397	234,708	140,950	169,995	515,622	6,346	6,124	14,877
21	Maine	280,593	4,668	53,161	19,679	13,446	11,058	59,867	550	1,154	922
22	Maryland	723,851	18,402	141,332	47,886	25,784	49,043	122,215	1,006	1,805	1,928
23	Massachussetts	629,620	5,371	120,973	38,471	24,003	16,572	137,671	849	1,990	1,628
24	Michigan	1,815,696	47,148	391,689	193,691	72,216	186,170	395,945	2,750	6,545	4,905
25	Minnesota	1,581,401	146,811	265,594	379,987	145,670	51,512	327,443	4,148	6,254	8,219
26	Mississippi	829,832	74,186	166,467	243,823	74,998	108,395	198,247	3,124	2,571	6,988
27	Missouri	1,821,503	112,168	359,925	465,919	151,192	174,688	381,758	6,486	4,701	10,161
28	Montana	573,472	27,679	111,261	241,293	69,323	26,005	186,424	3,017	2,019	6,177
29	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