



Emissions Inventory Preparation for Air Quality Modeling (Base Year)

July 29, 2019

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



Goals of Class

- ▶ To introduce you to the various tasks involved with preparing emissions inputs to air quality models
 - Focus is on the steps and data involved, not the details of running the scripts
- ▶ To answer commonly asked questions about emissions modeling
- ▶ Note: presentation is available for download:
<ftp://newftp.epa.gov/Air/emismod/training/>

Course Outline and Schedule



- ▶ 8:00 Background, Inventories, Tools, and QA
- ▶ 8:40 Emissions Modeling and Plume Rise
- ▶ **9:10 Break**
- ▶ 9:20 Temporal Allocation
- ▶ 9:40 Spatial Allocation
- ▶ 10:00 Speciation
- ▶ **10:20 Break**
- ▶ 10:30 Fugitive Dust, Biogenics, and Fires
- ▶ 10:55 Onroad and Commercial Marine Vessels
- ▶ 11:20 Final processing and QA steps
- ▶ **11:35 LUNCH**

Background: Purpose and Contents of a Modeling Platform

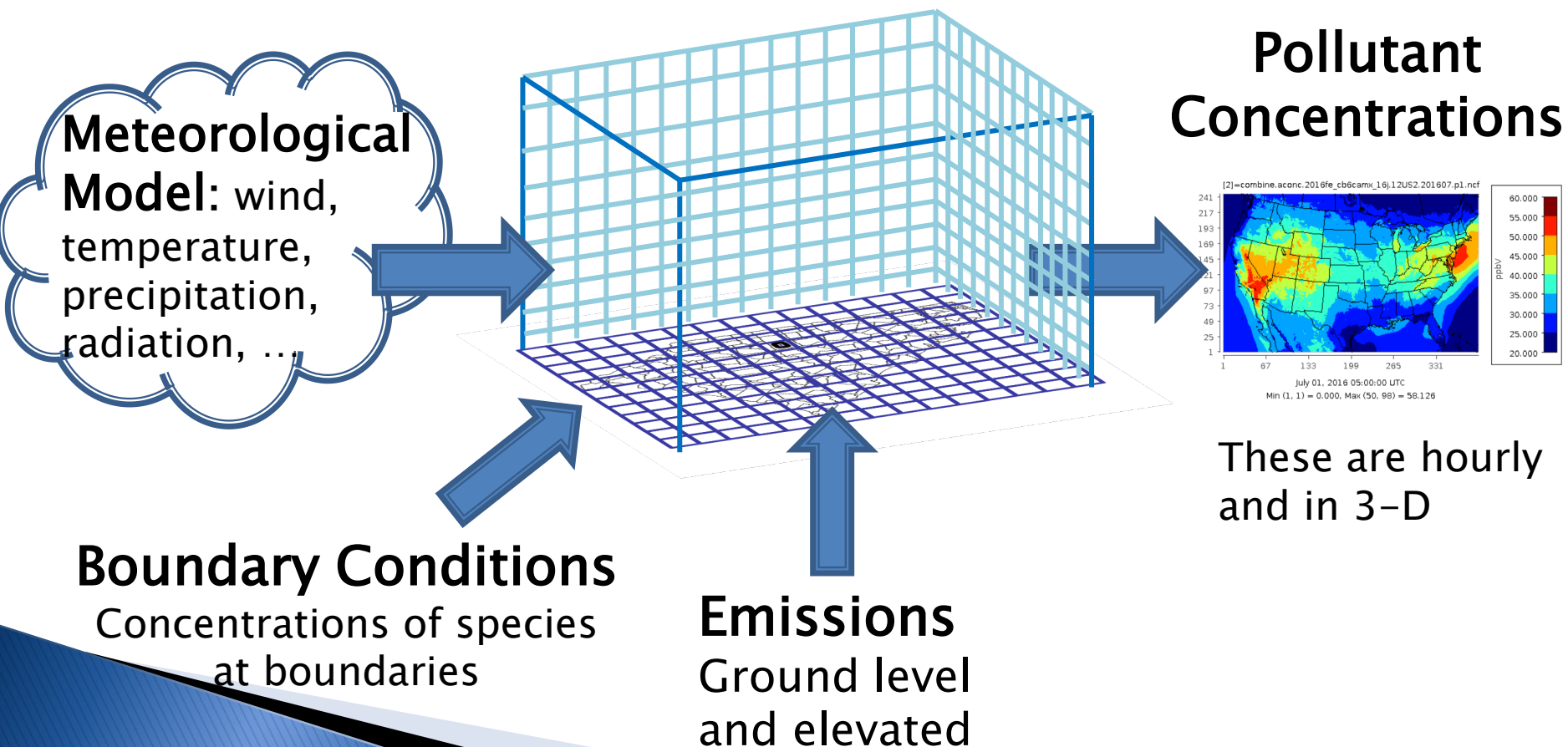


- ▶ Air quality modeling platforms are used to support air quality studies
 - Use technically sound data and state-of-the-science tools
- ▶ Major components of a modeling platform:
 - Meteorological models (WRF) and met. data
 - Boundary conditions (GEOS-Chem/Hemispheric CMAQ)
 - Air quality models (CMAQ, CAMx)
 - **Emissions:** base year (NEI)+NonUS, future year projections
 - **Other:** ancillary data for emissions modeling, projections data, emissions modeling tools (SMOKE, etc) and scripts

Air Quality Modeling Platform Components



Air Quality Model



Why do Air Quality Modeling?



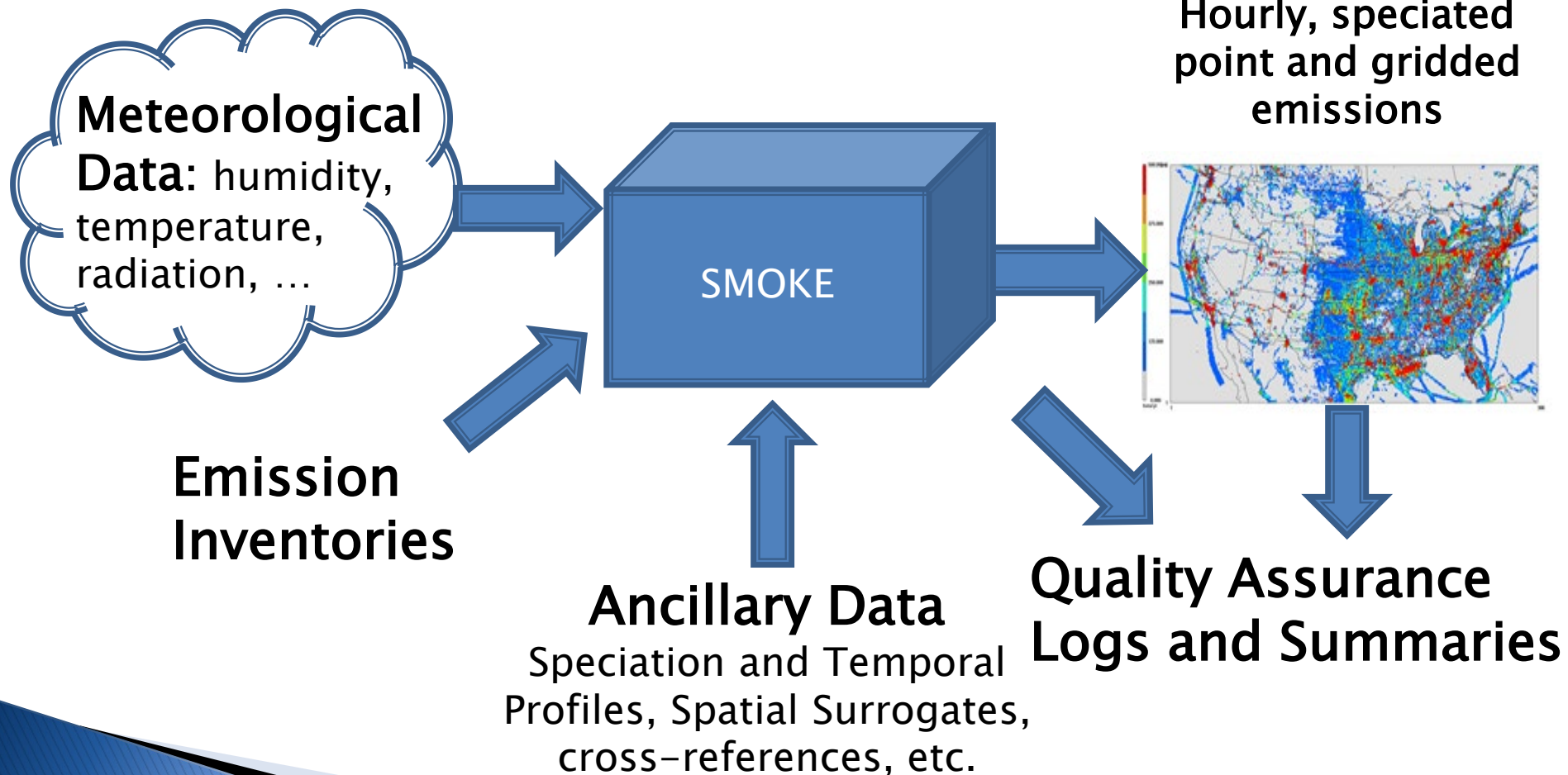
- ▶ **Regulatory Impact Assessments (RIAs)**
 - Model a base year focused on **Criteria Air Pollutants (CAPs)**
 - Model a future year base case with on-the-books rules
 - Model one or more cases that represent the rule
 - Estimate costs and benefits of rule
- ▶ **National Air Toxics Assessment (NATA)**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

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://www.cmascenter.org/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, NO₂, 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

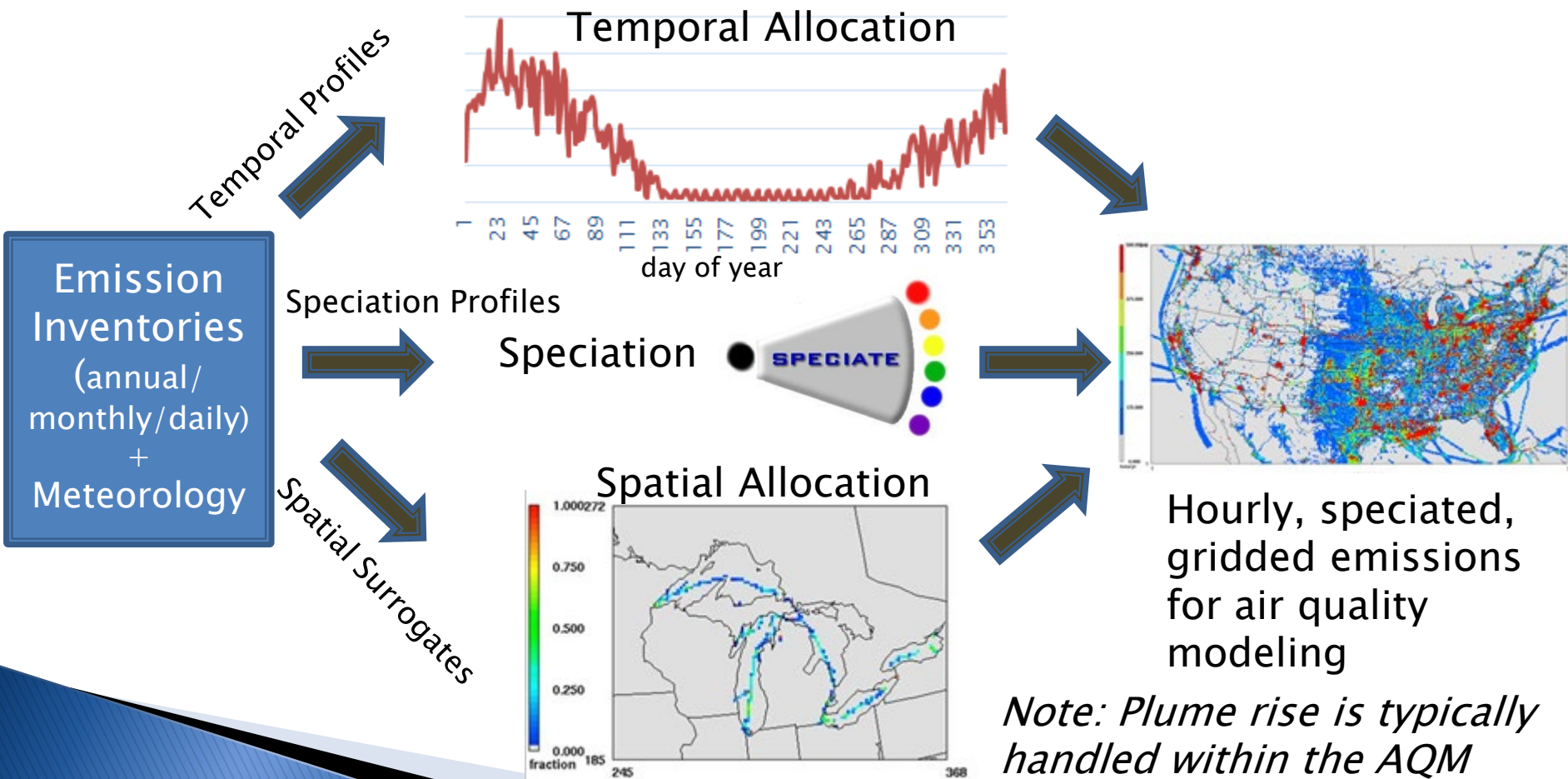
Emissions Modeling Schematic



Emissions Modeling Process



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



Base Year Emissions from the National Emissions Inventory (NEI)



- ▶ Data are submitted by states, locals, tribes (S/L/T) and EPA into the Emissions Inventory System (EIS)
- ▶ Five NEI data categories – all annual totals except events
 - Point/Facility Inventory (lat–lon locations): EGUs, airports, point oil and gas sources, commercial and industrial facilities
 - Nonpoint (county–based) – fugitive dust, agricultural, residential, industrial/commercial fuel comb., gas stations, biogenic
 - Onroad mobile sources (county): cars and trucks driving on roads
 - Nonroad mobile sources (county): mobile sources not on roads including rec. marine, construction equip., lawn/garden, tractors
 - Events (lat–lon, day): wildland and prescribed fires





NEI Compilation and Schedule

- ▶ EPA and S/L/T data are blended to create the NEI
- ▶ Full NEI produced every third year (e.g., 2011, 2014, 2017, 2020)
 - NEI Submissions due by end of the following year
 - 2014 NEI data due end of 2015; 2017 data due end of 2018
 - EPA compiles the inventory within about a year of submission
 - 2014NEIv1 released September, 2016
 - 2017NEI to be released as data categories are ready starting summer 2019 through spring 2020 (no v2 planned)
 - “Type A” (large) point sources submitted every year
 - 2016 sources due 12/31/17 (plus 2 week grace period)
- ▶ See <https://www.epa.gov/air-emissions-inventories>



Emissions Modeling Platforms

▶ Contents:

- Starting point is a version of the National Emissions Inventory (e.g., 2014 NEI version 2)
- Related data sets needed for processing are also included
- Software and scripts that process inventories into AQM inputs
- Typically have a historic or “base” year and one or more future years

▶ Historic platform development process:

- Base and future year inventories and met. data developed by EPA
- Data and software needed to process the inventories for AQM developed by EPA
- Platform released for public comment
- EPA incorporates comments into a new version of the platform

REPEAT



▶ Now applying a more collaborative process

Origins of the 2016 Platform Inventory Collaborative



- ▶ There were several versions of the 2011 platform created over multiple years (2013–2017)
- ▶ A new platform was needed based on 2014NEIv2
 - Needed for State Implementation Plans, Federal analyses
 - However, the year 2014 did not have much ozone
- ▶ The 2016 base year was selected for air quality modeling via a collaborative process among EPA, regional modeling groups and states
- ▶ Regional modeling organizations and states ***asked to be more involved*** in developing the next emissions platform
 - They wanted more input into the methods used, especially related to the “projections” of emissions to future years
 - In fall of 2017, regional modeling leaders and EPA *worked together* to prepare an 18 page development plan that laid the groundwork for the Inventory Collaborative effort



Organizational Structure

- ▶ **Coordination co-leads**: Zac Adelman (LADCO) and Alison Eyth (EPA OAQPS)
 - Developed process and communication structures, facilitate discussions, help resolve issues, documentation requirements, coordinate distribution of data to stakeholders
- ▶ **12 Sector-specific Workgroups**: each led by one regional/state staff and one EPA staff (where possible)
 - Prepare emissions estimates for 2016 and future years
 - Workgroups meet monthly; improve how the sectors are modeled
 - Include participants from EPA/states/locals/regions
- ▶ **Coordination committee**: regional, state, EPA leaders
 - Includes overall and workgroup co-leads plus MJO directors
 - Define processes, resolve issues, co-lead workgroups



Collaborative Workgroups (co-chairs)

- ▶ EGUs: Julie McDill (MARAMA), Serpil Kayin (CAMD), Alison Eyth
- ▶ Non-EGU Point: Caroline Farkas, Tammy Manning (NC)
- ▶ Nonpoint: Caroline Farkas, Jennifer Snyder (EIAG)
- ▶ Oil and gas sources: Jeff Vukovich, Tom Richardson (OK)
- ▶ Onroad: Alison Eyth, Julie McDill (MARAMA)
- ▶ Nonroad: Sarah Roberts (OTAQ)
- ▶ Rail: Mark Janssen (LADCO)
- ▶ Commercial Marine Vessels: Mark Janssen, NEI CMV leads
- ▶ Fires: Jeff Vukovich, past co-chair was Tom Moore (WESTAR)
- ▶ Biogenics: Jeff Vukovich, Doug Boyer (TCEQ)
- ▶ International: Alison (not a full-fledged workgroup)
- ▶ Modeling: Zac Adelman (LADCO), Eric Zalewsky (NY)
- ▶ Wiki has information about, and notes from, each workgroup
 - <http://views.cira.colostate.edu/wiki/wiki/9169>

2016 Platform Schedule

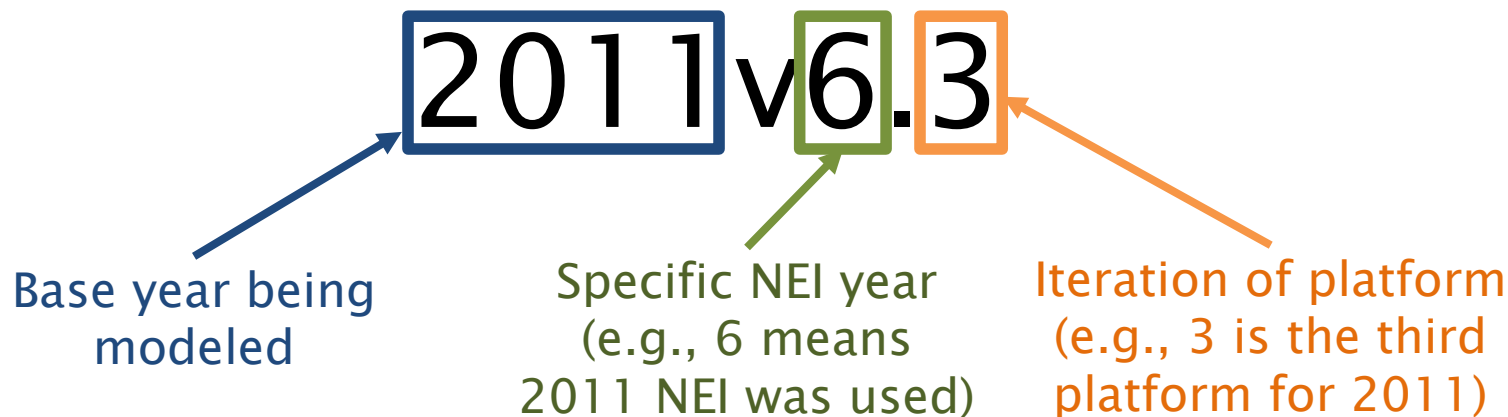


- ▶ Several versions of 2016 platform were planned
 - **Alpha:** *preliminary* version based on 2014NEIv2 for some and 2016 for other key sectors (released Spring, 2018)
 - For initial testing of 2016 model runs
 - **Beta:** *improved and/or new* version of 2016 emissions for all sectors (March 2019) **including inputs from states**
 - Preliminary projected emissions for 2023 and 2028 (April)
 - See <http://views.cira.colostate.edu/wiki/wiki/10197>
 - **V1.0:** *fully updated* 2016 emissions and complete projected emissions for 2023 and 2028 (late Summer 2019)
 - Can use some data available due to 2017 NEI

Recent Emission Modeling Platforms and Naming Convention



- ▶ 2011v6.3 platform is based on updated 2011NEIv2

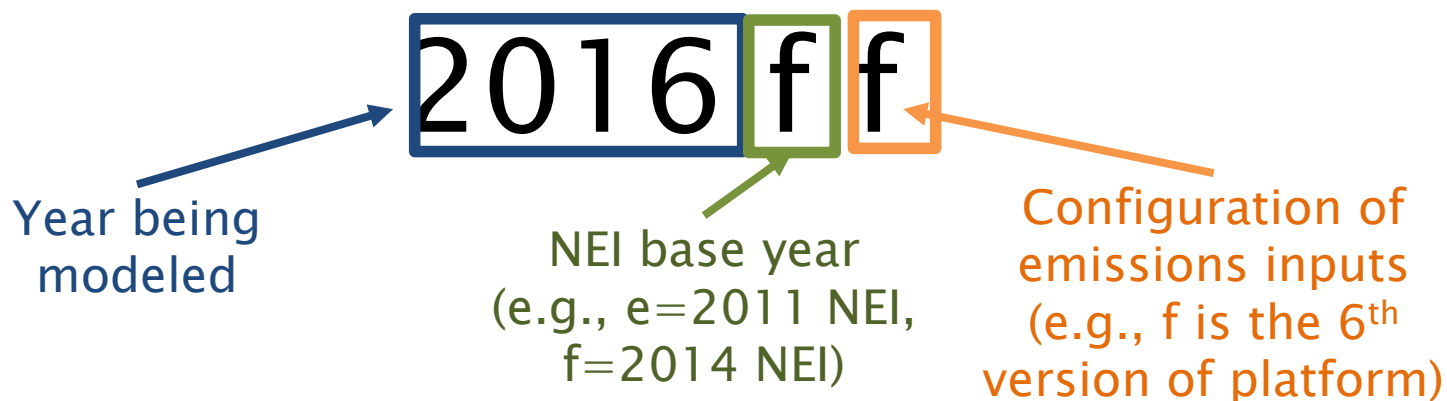


- Emission modeling platforms have base years and can have future years that go with them (e.g., 2023, 2028)
- ▶ 2014v7.1 was the 2014 NATA modeling platform based on 2014NEIv2
- ▶ 2016 Platform is currently under development and uses another nomenclature: alpha=7.1, beta=7.2, v1.0=7.3)



Emissions Modeling Case Abbreviations

- ▶ A “case” is a specific set of AQM–ready emissions inputs and has an abbreviation or nickname



- ▶ Additional information can follow the main abbreviation and differs by case
 - Speciation, control case, sensitivity adjustments, meteorological model configuration (e.g., 11g)
 - Such as cb6, ctl, nox50 (e.g., 2011ek_cb6_11g)

2014-16 Platforms Web Page



Case names appear on the web and FTP sites and in input file names

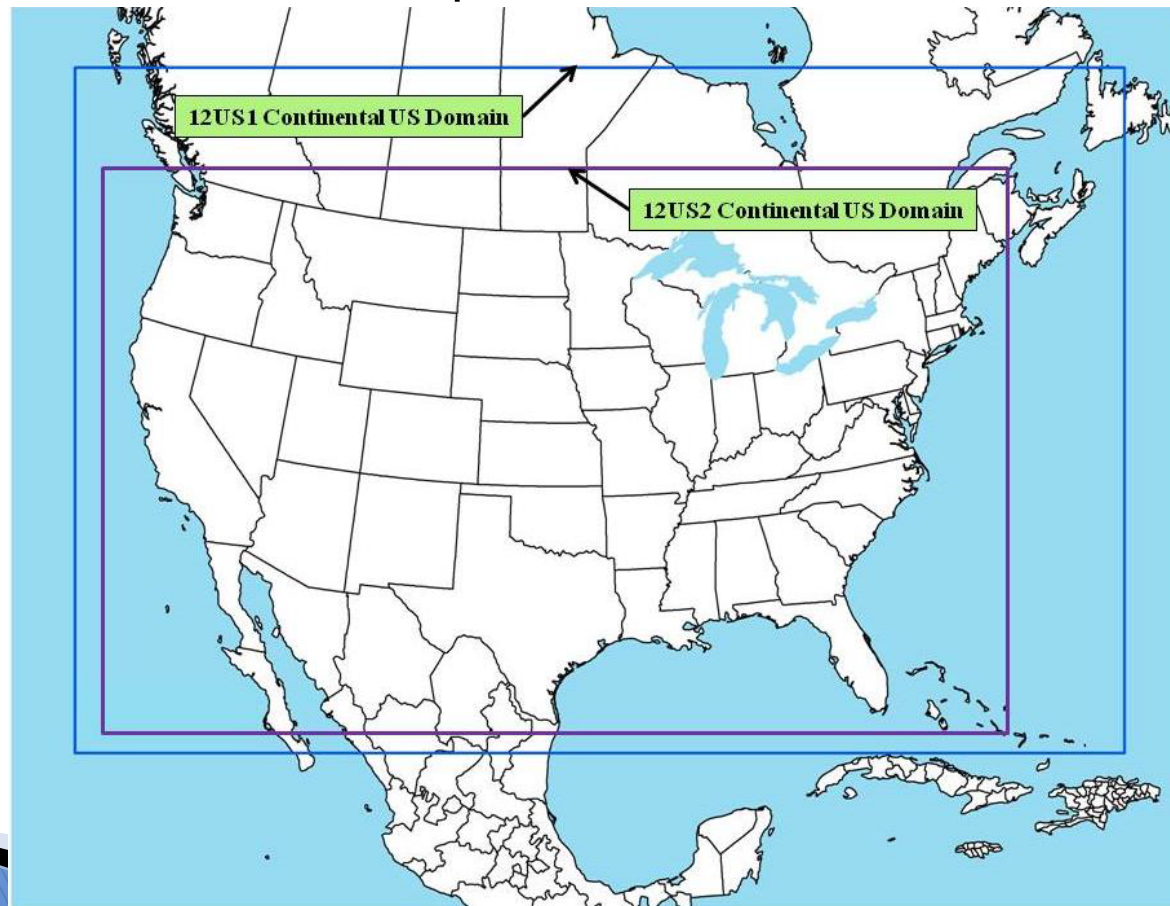
A screenshot of a web browser displaying the EPA website. The address bar shows the URL: https://www.epa.gov/air-emissions-modeling/2014-2016-version-7-air-emissions-modeling-platforms. The page title is "2014-2016 Version 7 Air Emissions Modeling Platforms". The main content area includes a description of the platforms and a list of links to specific versions: 2014v7.1 Platform, 2015v7.1 (alpha) Platform, 2016v7.1 (alpha) Platform, and 2016v7.2 (beta) Platform. The left sidebar contains navigation links for "Air Emissions Modeling/Home", "Emissions Modeling Platforms", "Emissions Modeling Tools", and "Training". The top navigation bar includes "Environmental Topics", "Laws & Regulations", and "About EPA". The bottom of the page has a "Contact Us" link and a timestamp of 5:36 PM.

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 platform

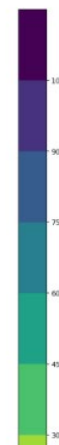
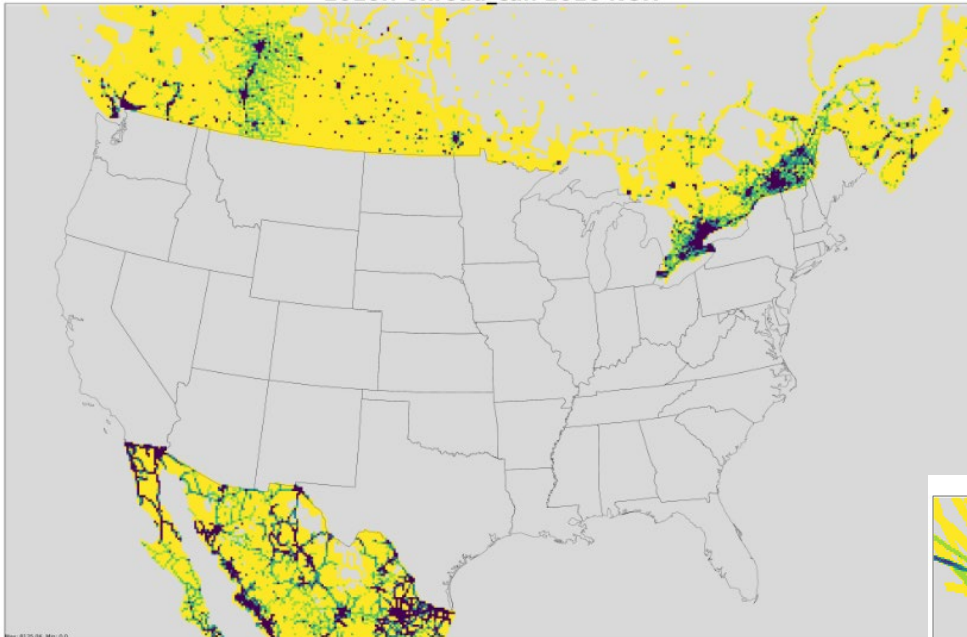


- ▶ Canada emissions & ancillary data (e.g., surrogates)
 - Courtesy Environment and Climate Change Canada
 - Most recent inventory is 2015 plus projection factors
 - Fire emissions provided for 2016 and other years
- ▶ Mexico 2008 emissions and projections of these
 - Based on Inventario Nacional de Emisiones de Mexico, 2008
 - MOVES–Mexico data was developed for key years
 - Base year fire emissions for Mexico derived from Fire INventory from NCAR (FINN):
 - A daily fire emissions product for atmospheric chemistry models [also used for winter in Canada]
- ▶ Hemispheric Transport of Air Pollution (HTAP) version 2 inventories used outside of North America in hemispheric runs

2016ff NOx Emissions Outside of the United States



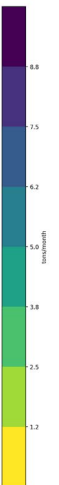
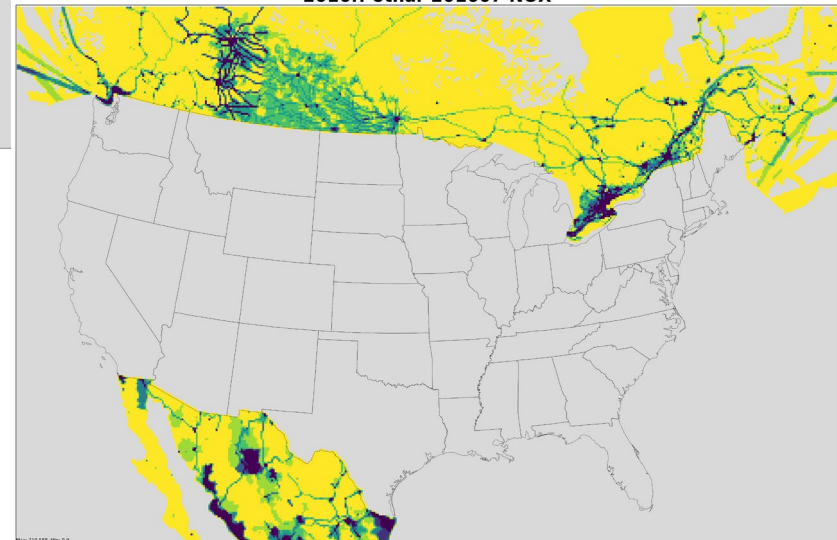
2016ff onroad_can 2016 NOX



Top: Onroad NOx emissions in Canada and Mexico

Bottom: Other (area) source NOx emissions in Canada and Mexico

2016ff other 201607 NOX



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 a lowercase name (e.g., rwc)
- ▶ Specific sectors vary by modeling platform but cover all sources in the inventory
- ▶ Point source sectors keep their specific latitude–longitude locations throughout the processing
- ▶ Nonpoint sectors are allocated to grid cells using spatial surrogates
- ▶ EPA processes emissions separately for each sector then merges the ground–level emissions together to create final AQM–ready files for a case

2016 Platform Sectors: Point and Non-U.S. (EPA platform)



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_othna	Non-US point source day-specific fires in North America
cmv_c3	Category 3 (large) Commercial Marine Vessels as points
othar	Non-US area (i.e., nonpoint) sources
othafdust	Non-US area fugitive dust sources (Canada only)
othptdust	Non-US point fugitive dust sources (Canada only)
othpt	Non-US point sources
onroad_can	Onroad mobile sources for Canada (was othon)
onroad_mex	Onroad mobile sources for Mexico (was othon)

2016 Platform Sectors: Ground-level



Nonpoint Sectors	Sector Description
afdust_adj	Met.-adjusted area fugitive dust emissions
ag	Agricultural emissions (primarily ammonia)
beis	Biogenic emissions based on the BEIS model
cmv_c1c2	C1&C2 Commercial marine vessels (nonpoint)
nonpt	Nonpoint sources not in other nonpoint sectors
nonroad	Mobile sources that do not drive on roads or railroads, including recreational pleasurecraft
np_oilgas	Nonpoint oil and gas production-related sources
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



Questions?

- ▶ Any questions on basic concepts of emissions modeling?



How do we Start Building a New Platform?



- ▶ **When a new NEI version becomes available, flat files** (a .csv format) are output from EIS
 - Point and nonpoint inventories are split into sectors
 - Onroad, nonroad, and biogenic are inputs to the NEI release
- ▶ Update ancillary files to account for new source classification codes (SCCs) and updated data
- ▶ Perform quality assurance as needed (temporal, speciation, gridding)
- ▶ **Compare the inventories and results to a previous platform**
 - Create difference reports by state, county, and/or SCC
 - Create charts and maps
 - Example: 2016 platform development



2014 vs 2016 Comparison

- ▶ First, prepare excel workbook by sector, state, pollutant, case 1, case 2, absolute and percent changes; then apply filters to prioritize (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	61%
ptagfire	California	PM2_5	3,596	5,689	2,093	58%
ptagfire	Florida	PM2_5	3,632	3,676	44	1%
ptagfire	Georgia	PM2_5	2,090	1,587	-503	-24%
ptagfire	Kansas	PM2_5	10,861	18,385	7,525	69%
ptagfire	Missouri	PM2_5	1,640	2,368	728	44%
ptagfire	North Dakota	PM2_5	1,969	3,241	1,272	65%
ptagfire	Oklahoma	PM2_5	6,124	9,545	3,421	56%
ptagfire	Texas	PM2_5	4,401	5,815	1,413	32%
ptagfire	Washington	PM2_5	1,694	1,334	-359	-21%

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; ptnonipm due to leap year

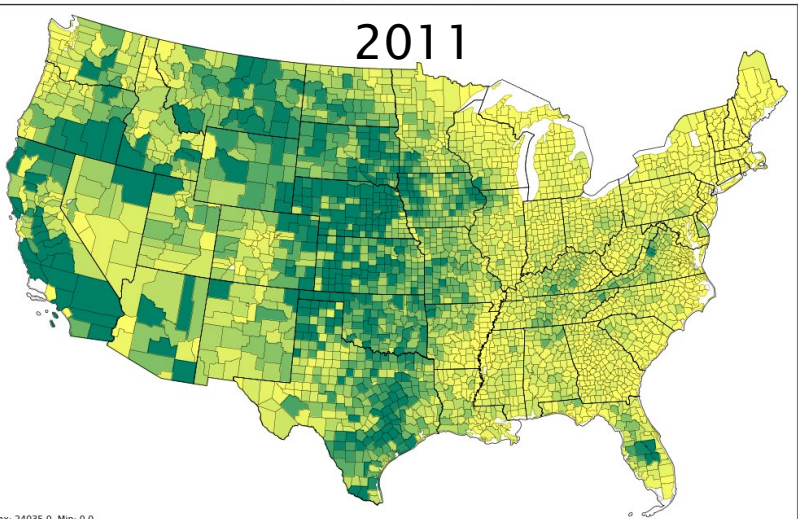
sector	state	county	poll	ann_emis_2014fb	ann_emis_2016fc	diff	pdiff
ptnonipm	Alabama	Autauga Co	CO	2,475	2,482	7	0.3%
ptnonipm	Alabama	Autauga Co	NH3	71	72	0	0.3%
ptnonipm	Alabama	Autauga Co	NOX	2,530	2,537	7	0.3%
ptnonipm	Alabama	Autauga Co	PM10	536	538	1	0.3%
ptnonipm	Alabama	Autauga Co	PM2_5	428	429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

County-level Base and Difference Maps: Beef Cattle NH₃



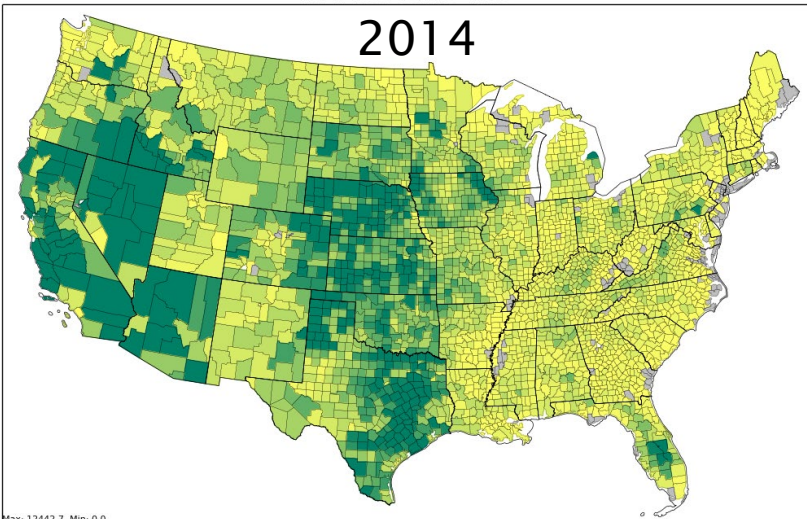
2011 Beef Cattle - NH₃

2011

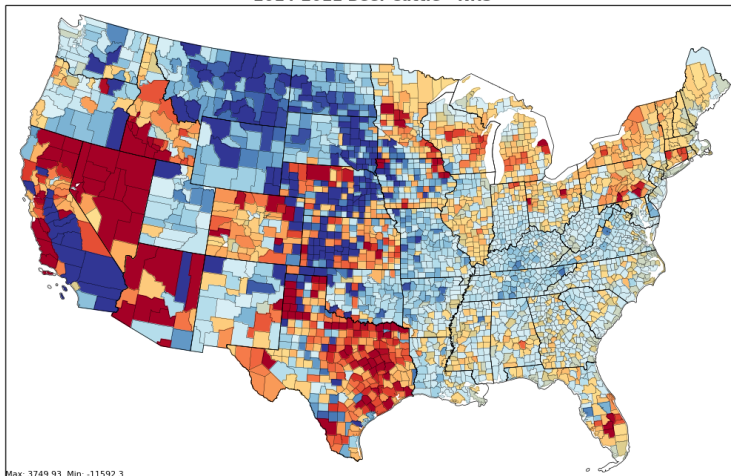


2014 Beef Cattle - NH₃

2014



2014-2011 Beef Cattle - NH₃



Maps help us see spatial variation and hot spots

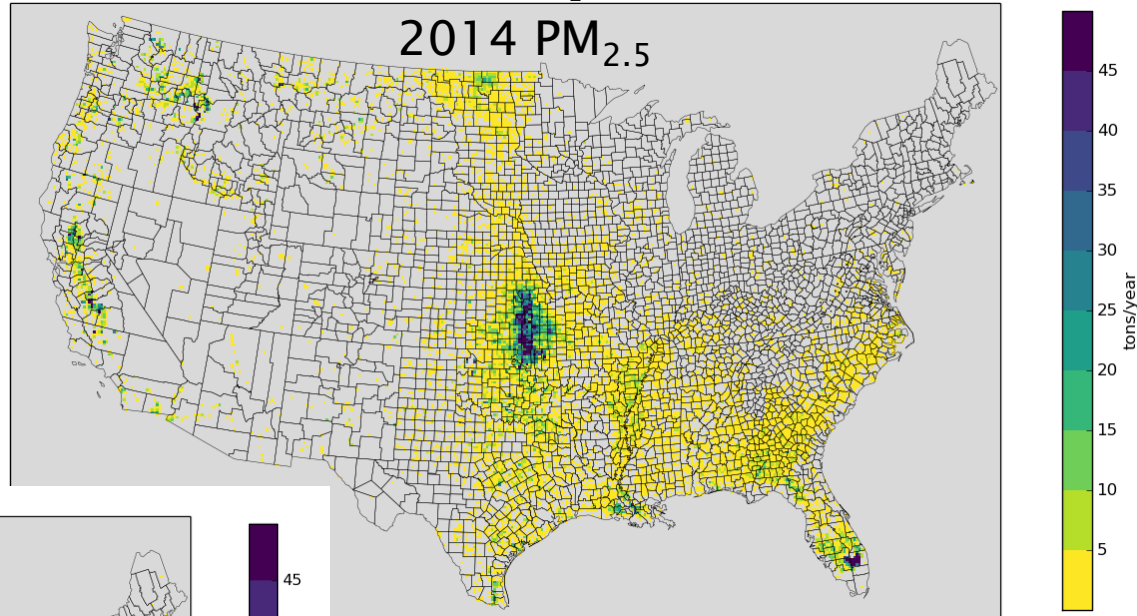
Most of our county-level maps are created with Python

Gridded Maps: Ptagfire Example

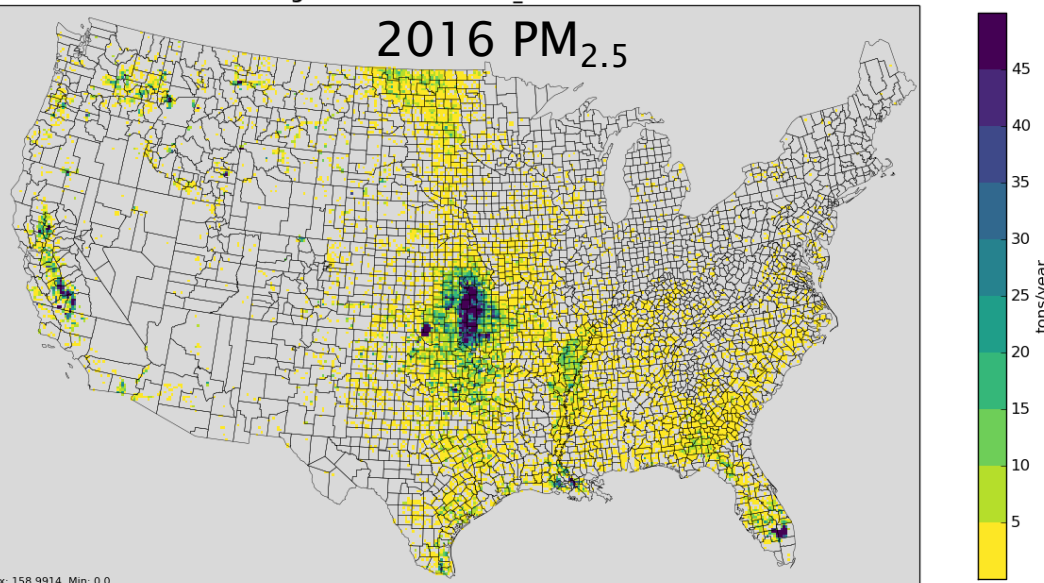


Gridded maps can be created with VERDI, PAVE, etc.

Point Agricultural Fires PM_{2.5} - Annual 2014



Point Agricultural Fires PM_{2.5} - Annual 2016



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

Modeling Platform Data is not always the same as the NEI



- ▶ Some modeling platform data 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
- ▶ For 2016 platform, lots of 2016-specific data are used and updated methods were developed



Questions?

- ▶ Questions on new platform development or quality assurance?



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



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 county emissions into grid cells
- ▶ Speciation Tool: creates chemical speciation profiles from SPECIATE database profiles (e.g., $\text{NO}_x \rightarrow \text{NO} + \text{NO}_2$, $\text{PM}_{2.5} \rightarrow \text{EC} + \text{OC} + \dots$, $\text{VOC} \rightarrow \dots$)
- ▶ 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



Emissions Modeling Framework (EMF): Alison Eyth (auv), Server

File Manage Window Tools Help

Dataset Manager

Show Datasets of Type: Flat File 2010 Point Name Contains: 2016 Refresh Advanced

#	Select	Name	Last Modified Date	Type	Sta
1	<input type="checkbox"/>	ptinv_ptfire_sf2_2016_ff10	2017/07/07 12:33	Flat File 2010 Point	Imported
2	<input type="checkbox"/>	ptinv_c3_cmv_point_2016_ff10	2017/06/27 16:48	Flat File 2010 Point	Imported
3	<input checked="" type="checkbox"/>	ptegu_2014NEIv1_final_POINT_for_2016fc	2017/06/12 10:07	Flat File 2010 Point	Imported

Dataset Properties View: ptegu_2014NEIv1_final_POINT_for_2016fc (ID = 455716)

Summary Data Keywords Notes Revisions History Sources QA

Name: ptegu_2014NEIv1_final_POINT_for_2016fc (ID = 455716)

Description: #FORMAT=FF10_POINT
#COUNTRY=US
#YEAR=2016
#SELECTION_NAME=2014 NEI FINAL V1
#INVENTORY_VERSION=General Purpose Release
#INVENTORY_LABEL=2014 NEI FINAL V1

Project:

Creator: Allan Beidler (abeidler)

Dataset Type: Flat File 2010 Point

Time Period Start: 01/01/2016 00:00	Status: Imported
Time Period End: 12/31/2016 23:59	Last Modified Date: 06/12/2017 10:07
Temporal Resolution: Annual	Last Accessed Date: 06/12/2017 10:11
Sector:	Creation Date: 06/05/2017 15:07
Region:	Intended Use: public
Country:	Default Version: 1 (remove unit)

Edit Properties Edit Data Refresh Export Close

Emission inventories are stored as Datasets in the Emissions Modeling Framework

EMF Showing Point Inventory (FF10)



Emissions Modeling Framework (EMF): Alison Eyth (auv), Server _____)

File Manage Window Tools Help

Data Viewer [Dataset:ptegu_2014NElv1_final_POINT_for_2016fc, Version: remove unit, Table: DS_ptegu_2014NElv1_final_POINT_for_2016fc_8584...]

Sort Order:

Row Filter: **ANN_VALUE > 10** Filter records using SQL

Apply

Current: 1 - 300 Filtered: 17193 of 253022

Decimal Places: 1 Show Commas Format Reset View

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	
US	01073	1003111	62941313	57680112	86652714	010730011	10100222	NOX	1,902.4	
US	01073	1003111	62941313	57680112	86652714	010730011	10100222	PM10-FIL	63.9	
US	01073	1003111	62941313	57680112	86652714	010730011	10100222	PM10-PRI	70.3	
US	01073	1003111	62941313	57680112	86652714	010730011	10100222	PM25-FIL	19.9	
US	01073	1003111	62941313	57680112	86652714	010730011	10100222	PM25-PRI	26.2	
US	01073	1003111	62941313	57680112	86652714	010730011	10100222	PMFINE	21.6	
US	01073	1003111	62941313	57680112	86652714	010730011	10100222	SO2	215.6	
US	01073	1003111	62941313	57680112	86652714	010730011	10100222	VOC	109.1	
US	01073	1003111	62941413	57680212	86652814	010730011	10100222	CO	691.8	
US	01073	1003111	62941413	57680212	86652814	010730011	10100222	NOX	1,599.0	
US	01073	1003111	62941413	57680212	86652814	010730011	10100222	PM10-FIL	60.8	

Add Note Close

Emissions Modeling Steps for Ground-level Sectors



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 Non-U.S. and Point Sectors



Platform sector	Spatial	Speciation	Inventory resolution	Plume rise
othafdust	Surrogates	Yes	annual	
othar	Surrogates	Yes	annual	
othpt	Point	Yes	annual	in-line*
othptdust	Point	Yes	monthly	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	in-line
ptnonipm	Point	Yes	annual	in-line
cmv_c3	Point	Yes	Annual	in-line

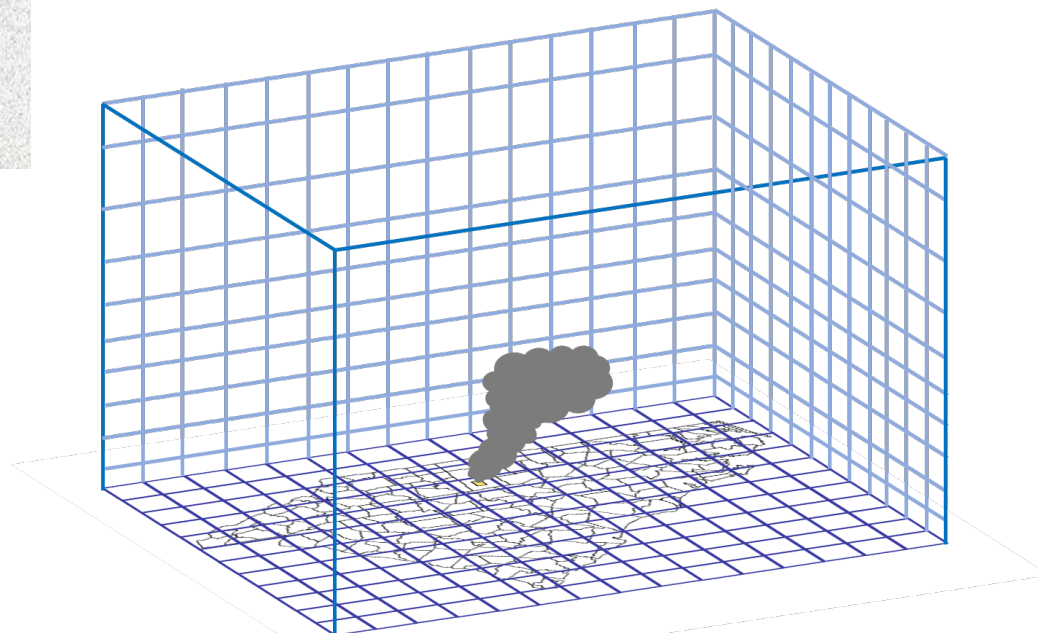
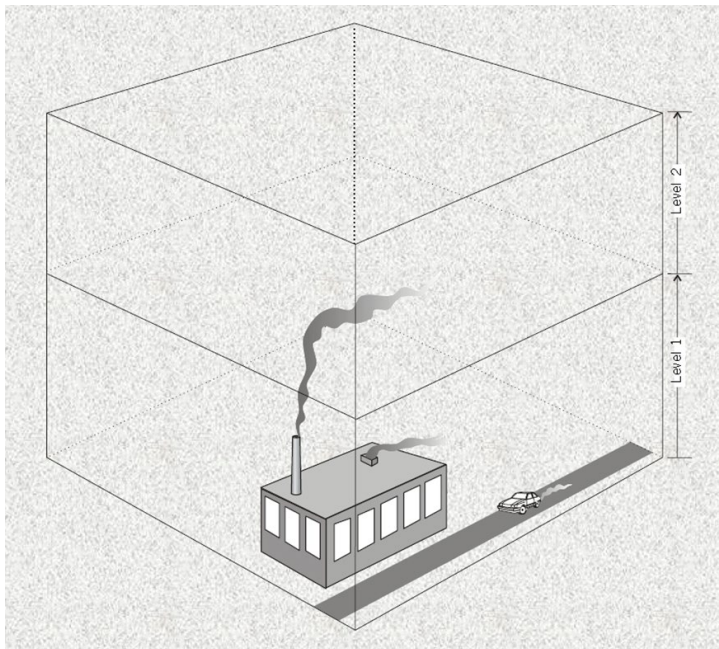
* in-line means the plume rise can be done in CMAQ



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 $> 20\text{m}$ 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 applications, 3-D emissions are developed

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
 - H_S = Physical stack height (m)
 - F = Buoyancy 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)

Plume Rise Requirements for AQMs Differ

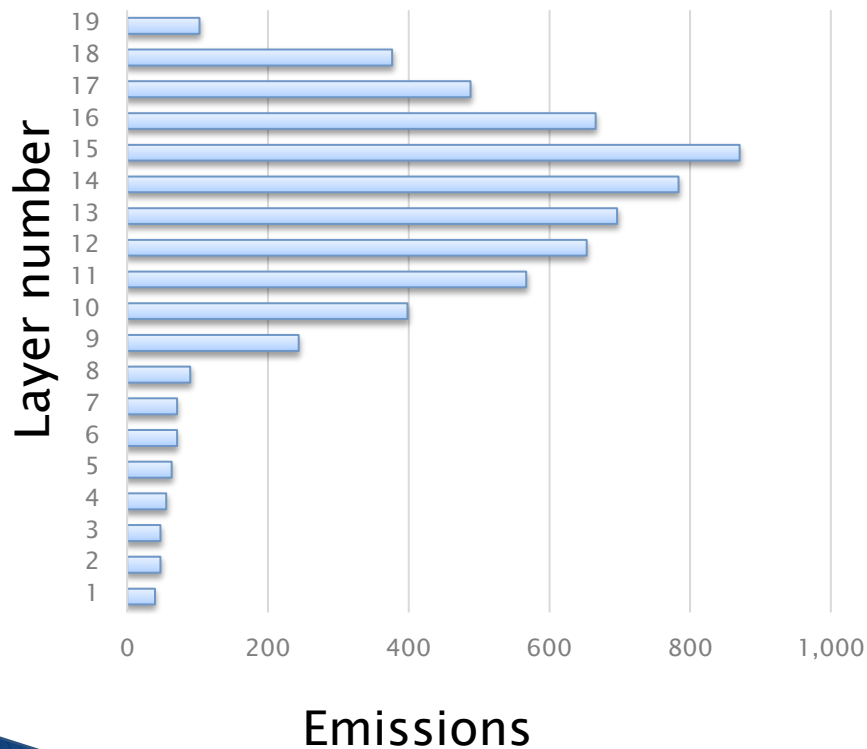


- ▶ 3-D emissions files can be really big!
- ▶ CMAQ can do “in-line” plume rise
 - Provide CMAQ with hourly emissions with locations and stack parameters for any elevated sources
 - Compute plume rise with hourly meteorological data
 - A special plume rise treatment is used for fires that considers acres 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



Example Fire Plume Rise





Questions?

- ▶ Any questions on SMOKE or plume rise?





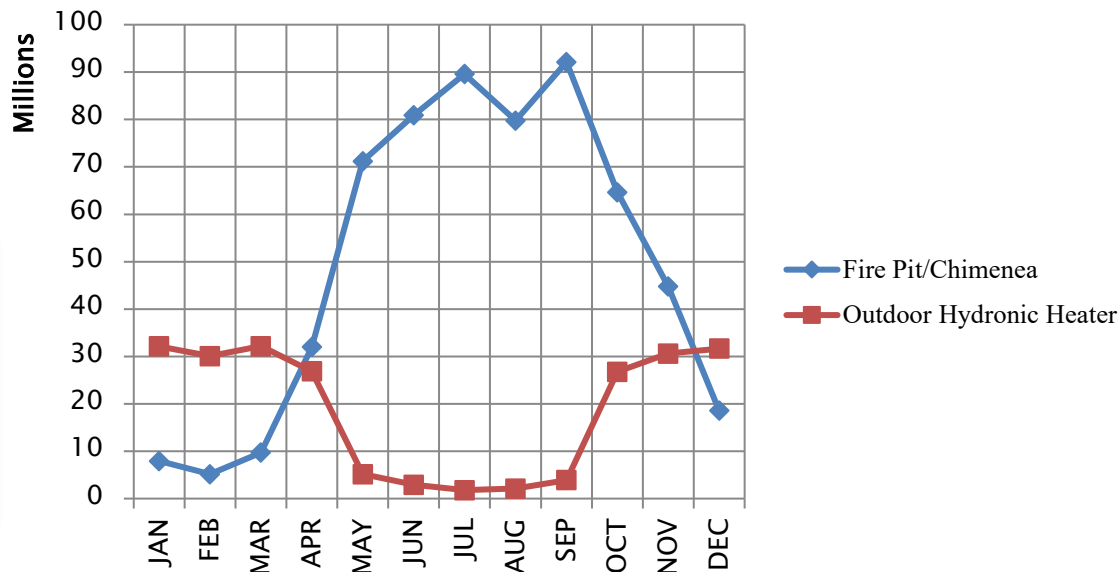
Temporal Allocation

- ▶ Temporal allocation is the process of allocating inventory emissions to hourly emissions
- ▶ Hierarchy of temporal allocation steps:
annual → month → day of week → hour of day
- ▶ 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 – no “packets” like old format

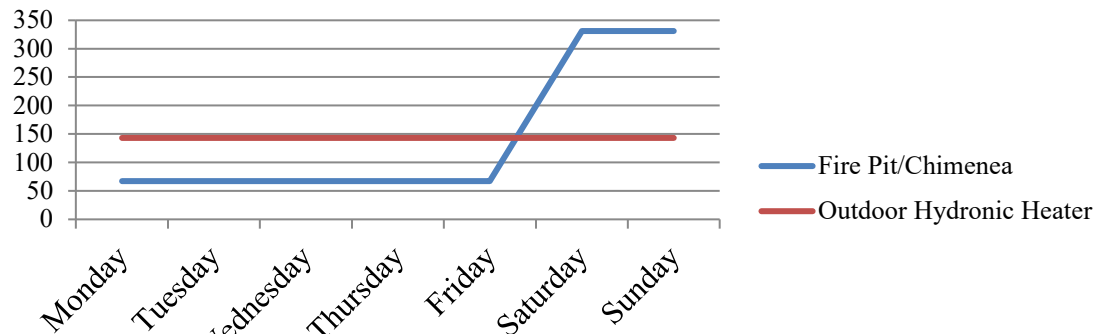
Temporal Profile Examples



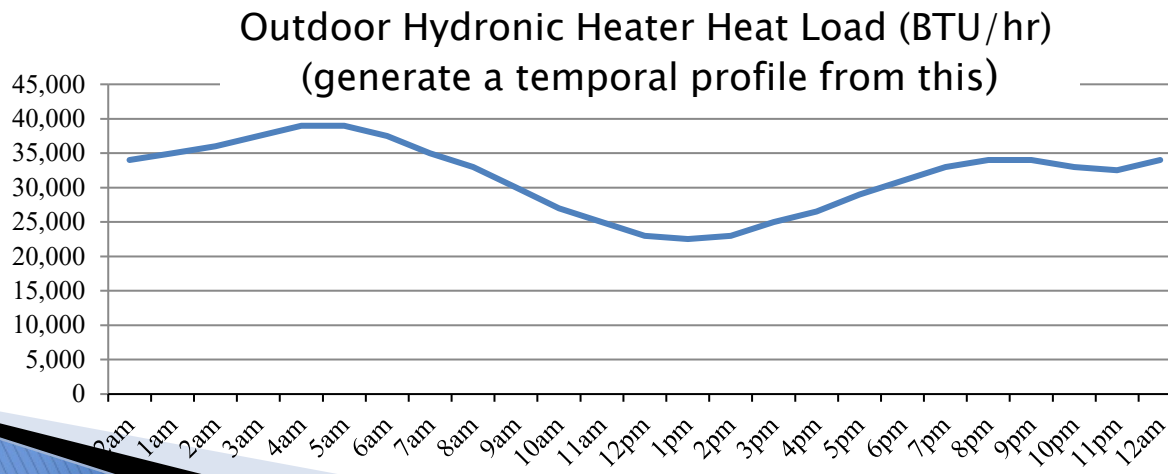
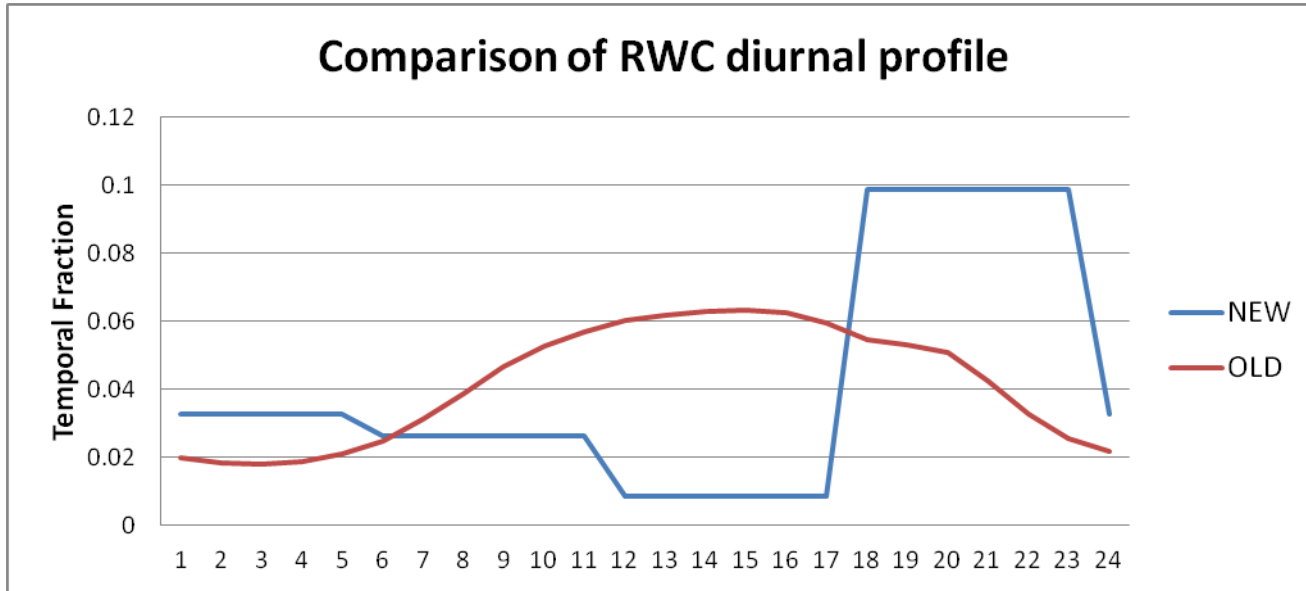
Monthly Temporal Activity for Outdoor Hydronic Heater & Recreational Residential Wood Combustion



Fire Pits/Chimineas Day-of-Week Profile



Diurnal Temporal Profile Examples



Excerpt from Temporal Cross Reference and Profile Files



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

Profiles

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	0.14	Equal	all days		
61500	0.07	0.07	0.07	0.07	0.07	0.33	0.33	Fire pit	higher	weekends		
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	0.05	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
ptagfire	Daily	No	all	all	Yes
beis	Hourly	No	n/a	all	No
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
othptdust	Monthly	No	mwdss	mwdss	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_othna	Daily	No	all	all	Yes
rwc	Annual	No	met-based	all	Yes



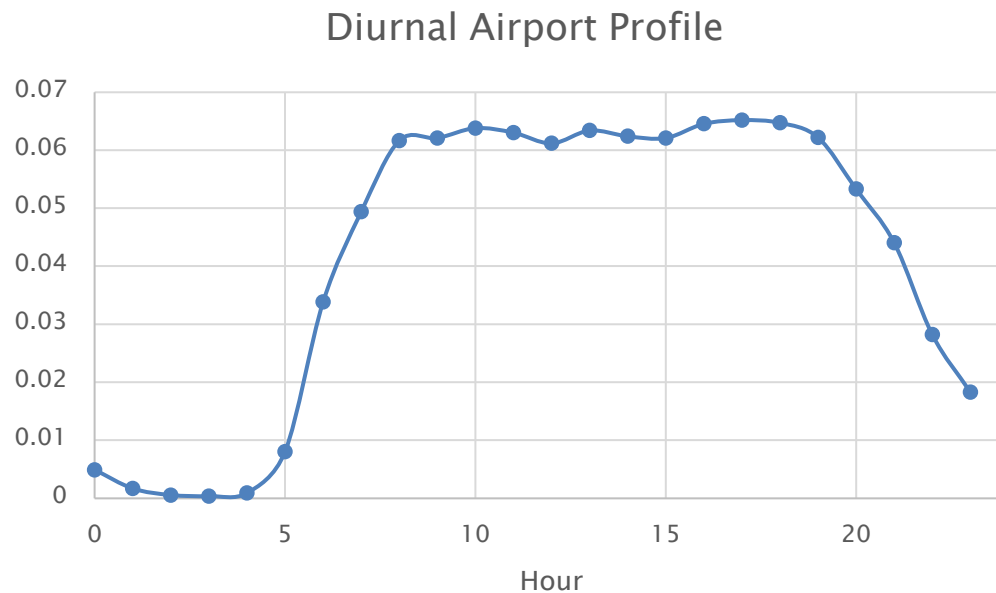
Temporal Profile Data Sources

- ▶ Some temporal profiles have been used for a while
- ▶ We look for data sources that can be used to update 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 updated
- ▶ 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>

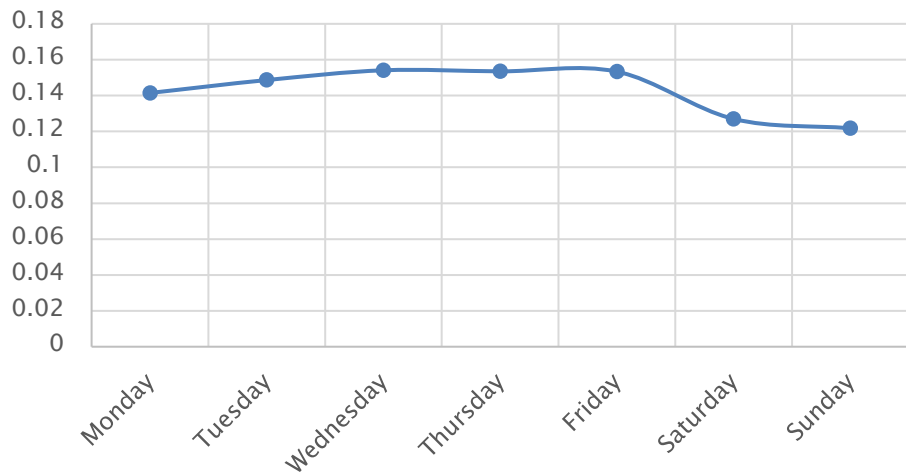




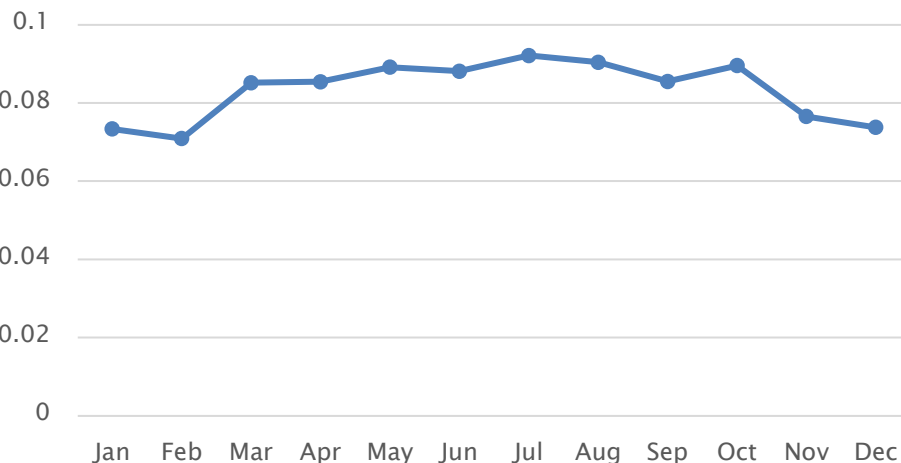
Airport Temporalization (2/2)

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

Weekly Airport Profile



Monthly Airport Profile

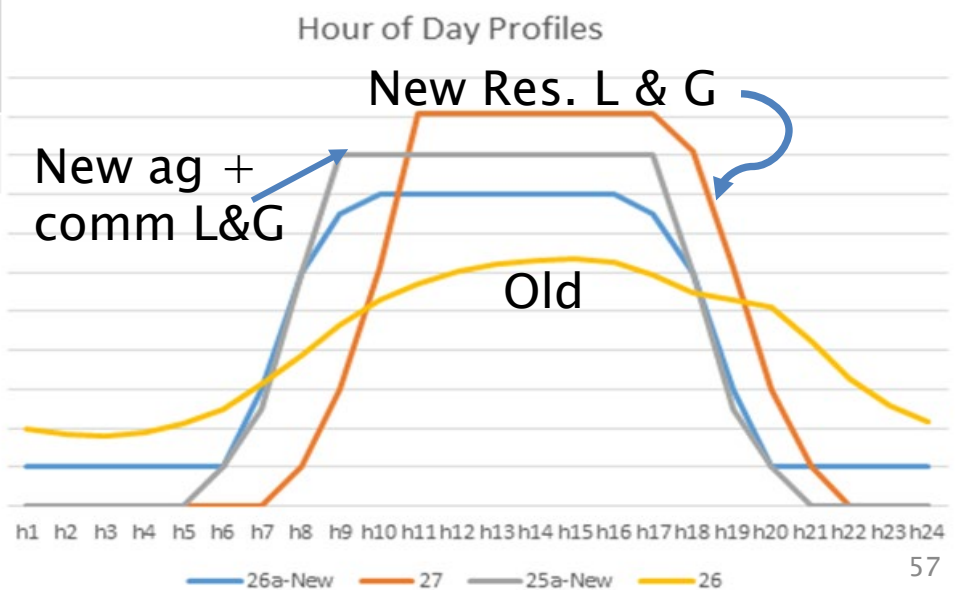
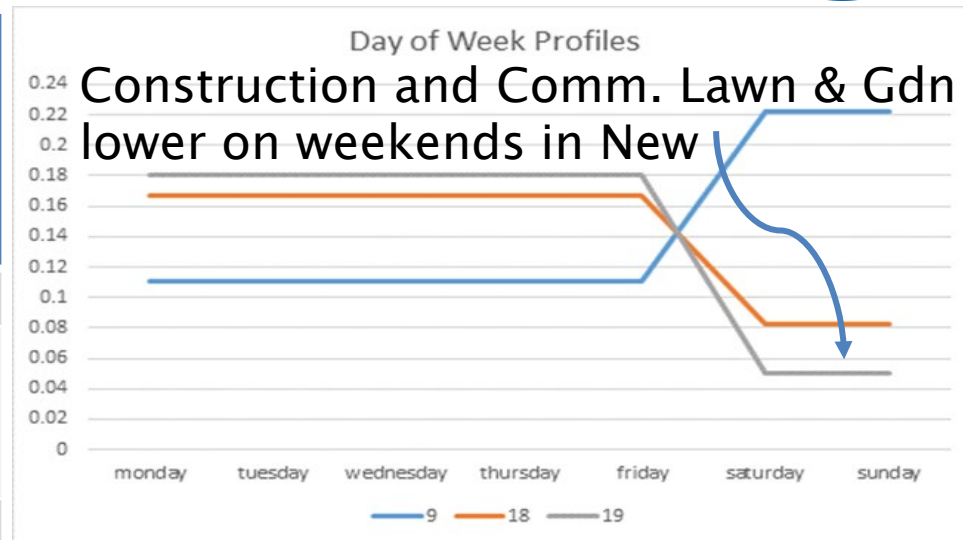


Nonroad Temporal Profile Updates



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





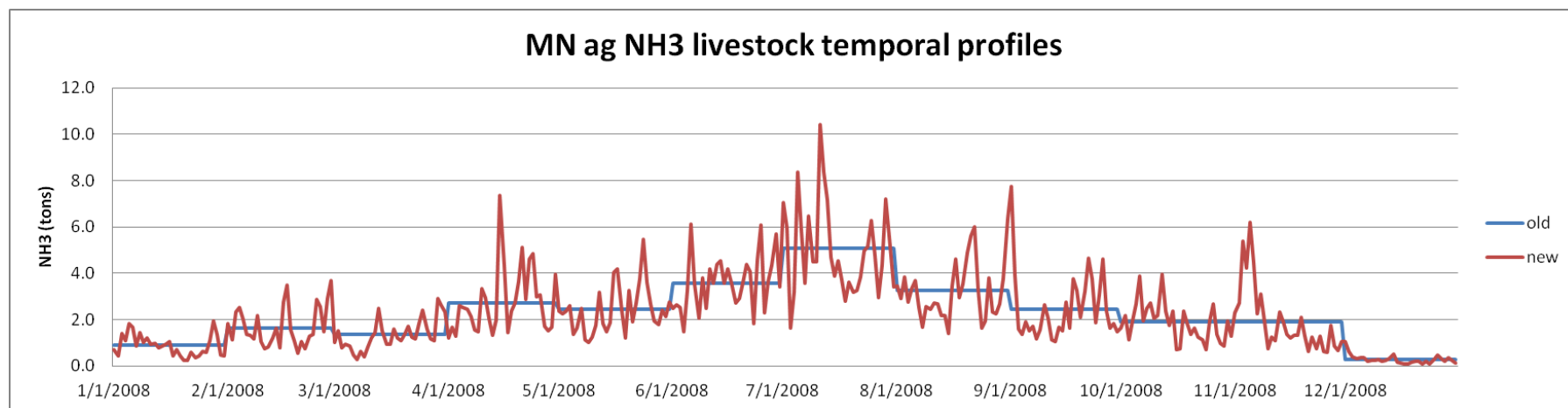
Meteorology-based Temporalization

- ▶ 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
 - Used for platform sectors: ag (month->hour) and rwc (annual->day of year)
- ▶ Other sectors influenced by meteorology
 - Area fugitive dust (afdust)
 - Biogenic emissions
 - Onroad (discussed later)
 - EGUs (indirectly)



GenTpro: ag livestock

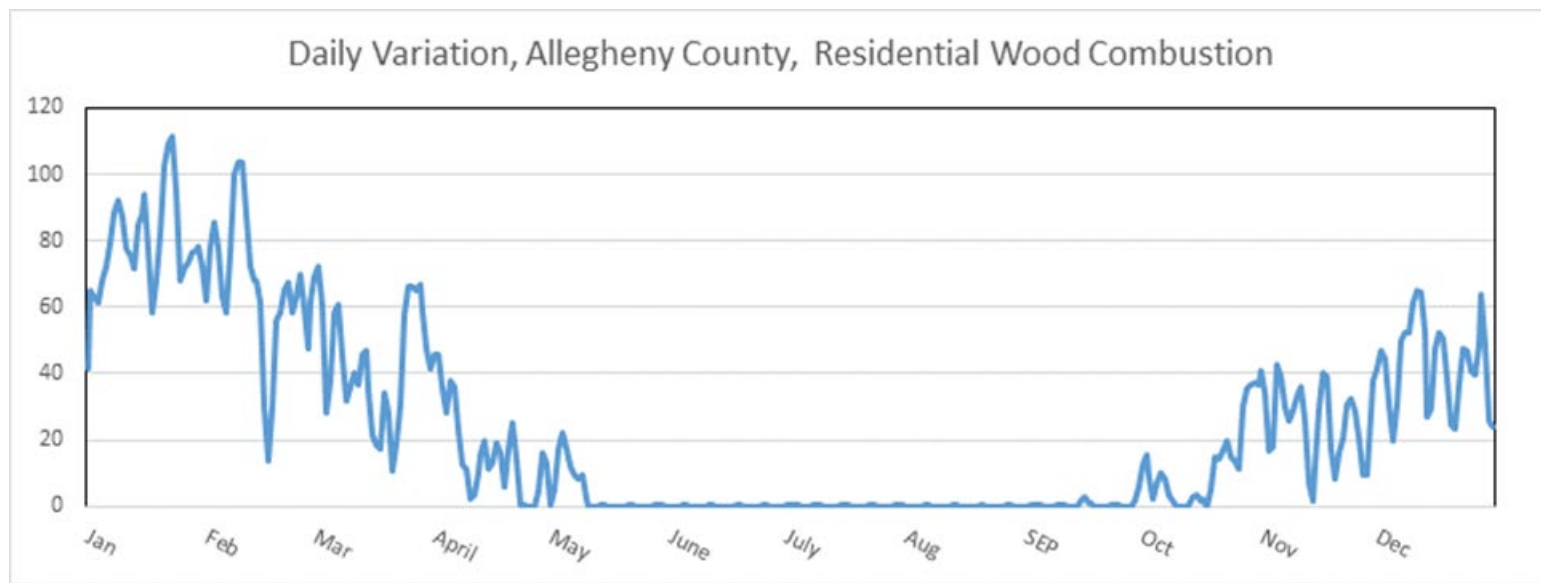
- ▶ Meteorological fields used: temperature, wind speed, and aerodynamic resistance
- ▶ Allocate monthly emissions to hour of month





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



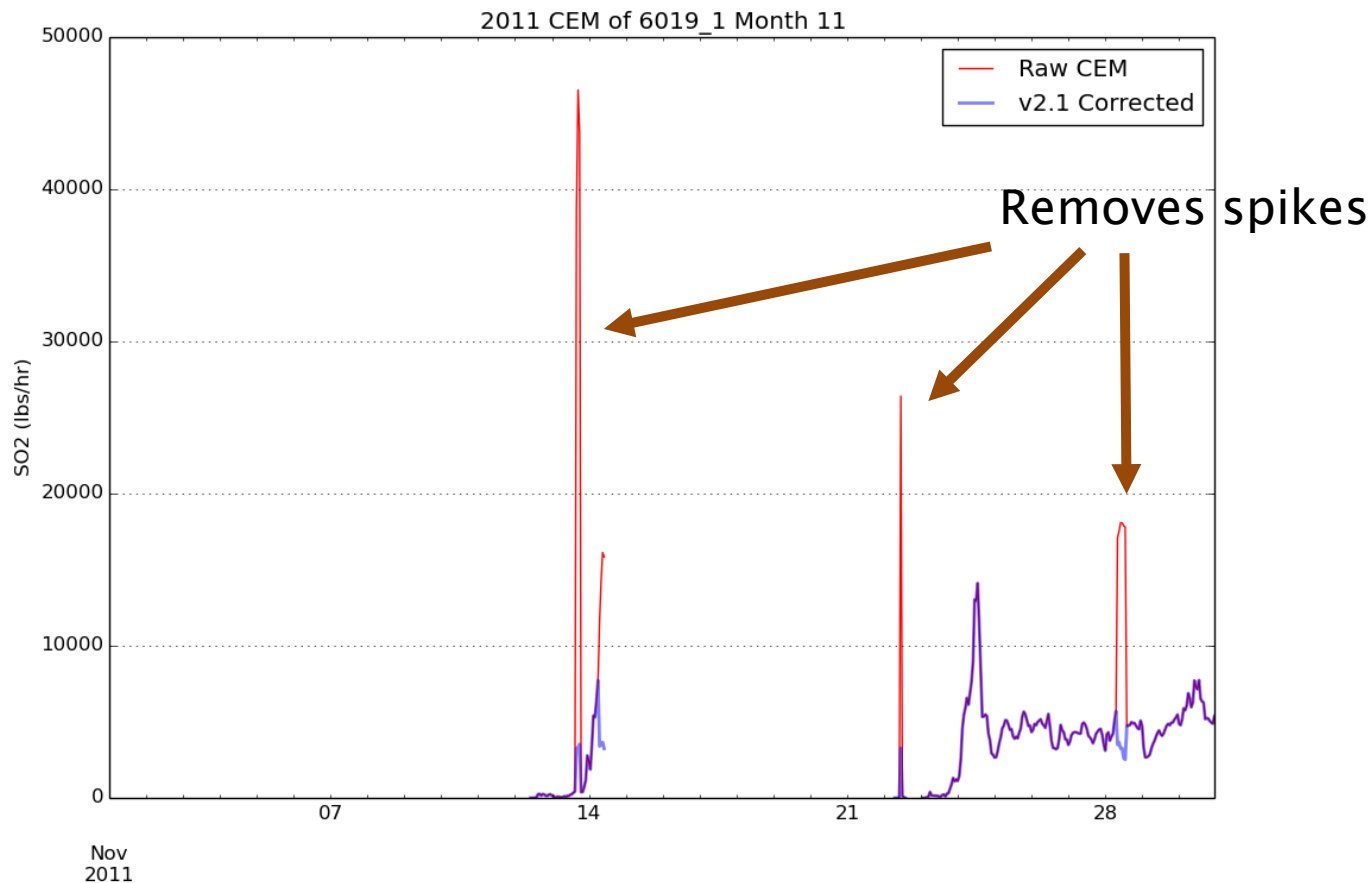
Special Steps Taken for EGUs



Future year emissions generated using Integrated Planning Model (IPM)

1. Separate EGUs from nonEGUs in EIS flat file based on whether IPM_YN column in flat file is non-blank
2. Download latest CEMS data for base year of interest
3. Review the assignments to ORIS IDs (used for CEMS) in the flat file and how they match up to the CEMS data
4. Identify partial year CEMS reporters; plus sources that should not use CEMS-based profiles (e.g., MWCs, cogens)
5. Run cemcorrect program to remove non-measured anomalies in CEMS data
6. Generate region/fuel-specific average temporal profiles for temporalization of sources without CEMS
7. Generate region/fuel-specific hourly profiles for winter and summer [and for peaking and non-peaking]

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

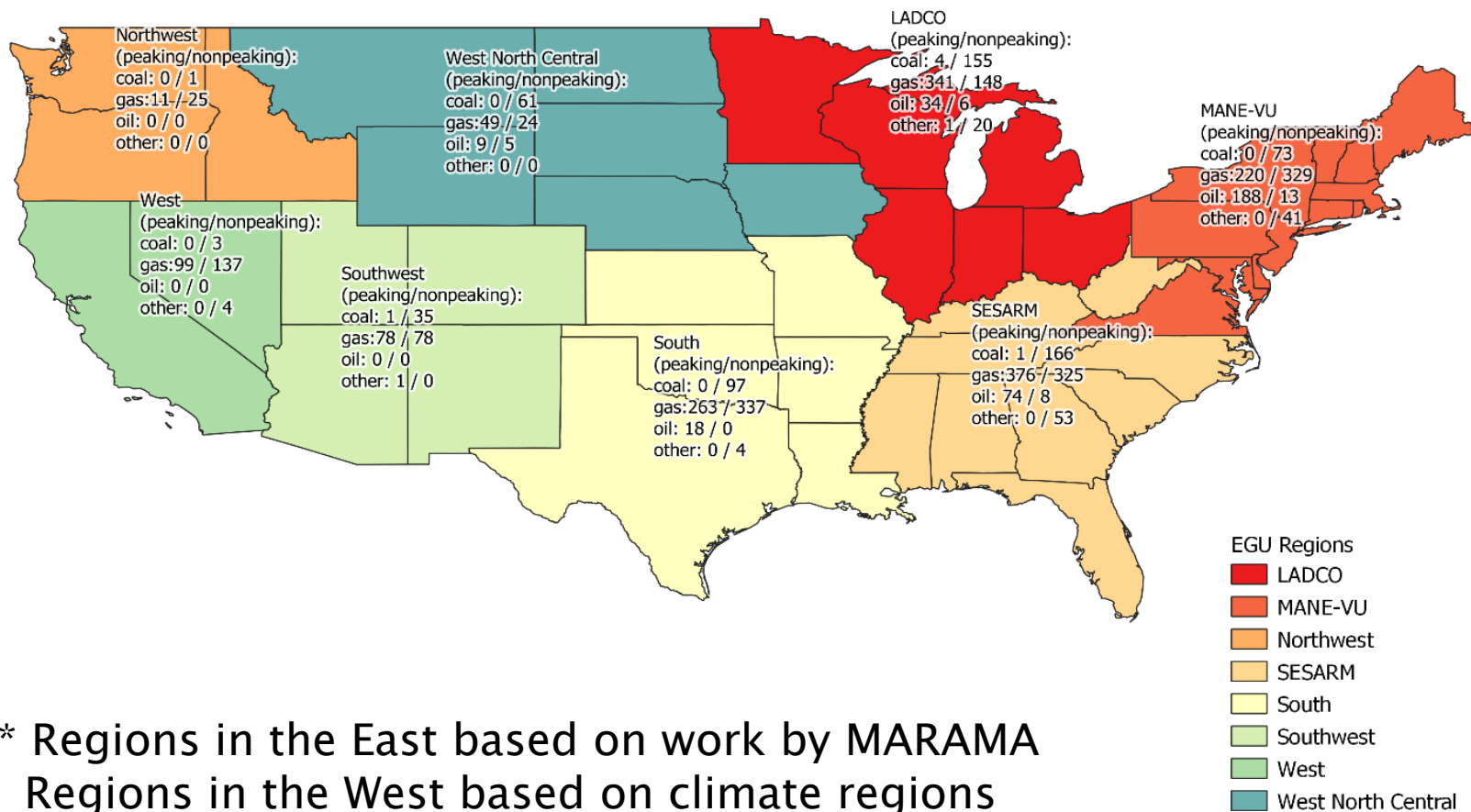


- ▶ Removed non-measured data values from CEMS data to ignore emission spikes
- ▶ Hierarchy of CEMS assignments:
 1. Use CEMS for all months (units with complete CEMS data)
←-- **Note: CEMS data replace the annual inventory**
 2. Partial year reporters use CEMS for months where there are measurements but use regional averages for periods without measurements [**Note: sources can differ by year**]
 3. Use regional averages (for units without CEMS)
- ▶ Regional average profiles for sources without CEMS
 - Region and fuel-specific average profiles used: peaking and non-peaking
 - Different winter and summer versions of hourly profiles
- ▶ Matching of CEMS database units and future year units with FIS/platform point sources is key to success

Map of EGU Temporal Regions



Small EGU 2016beta Temporal Profile Input Unit Counts

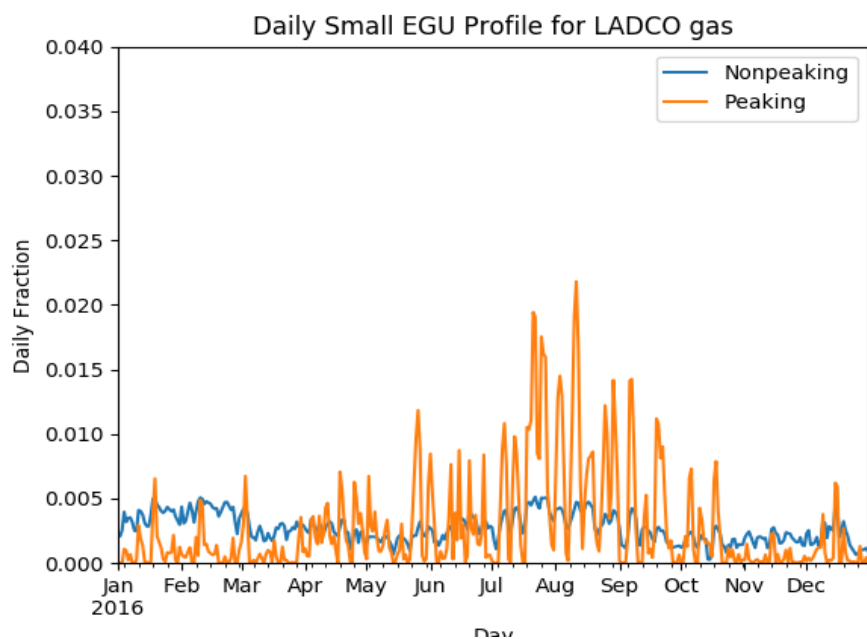


* Regions in the East based on work by MARAMA
Regions in the West based on climate regions

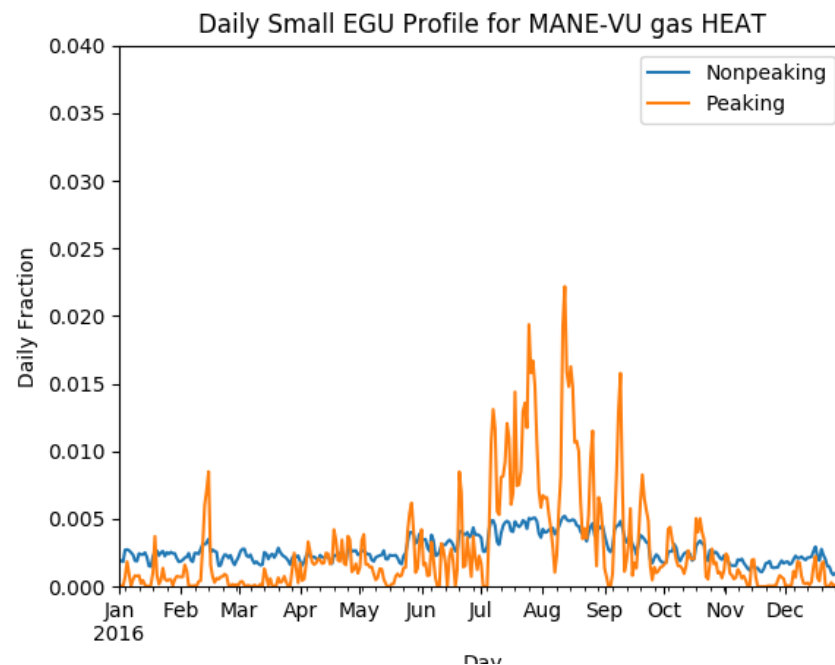
Average Month-day Profiles: Region- and fuel-specific



Profiles differ between regions
(orange=peaking, blue=non-peaking)



LADCO gas profiles



MARAMA gas profiles

Note: for 2016, profiles assigned by unit, not SCC



Identifying Peaking Units

- ▶ Peaking units have an annual capacity factor of less than 0.2 and a multiyear capacity factor of less than 0.1

or

less than 20% utilization in the base year and less than 10% utilization across a 3-year period, where:

- ▶ Base year (2016) annual capacity factor:
 - $(\text{annual unit output MWh}) / (\text{unit capacity MW} * 8760 \text{ h})$
- ▶ Multiyear (2014–2016) capacity factor:
 - $(3 \text{ year unit output MWh}) / (\text{unit capacity MW} * 3 * 8760 \text{ h} + 24 \text{ h})$

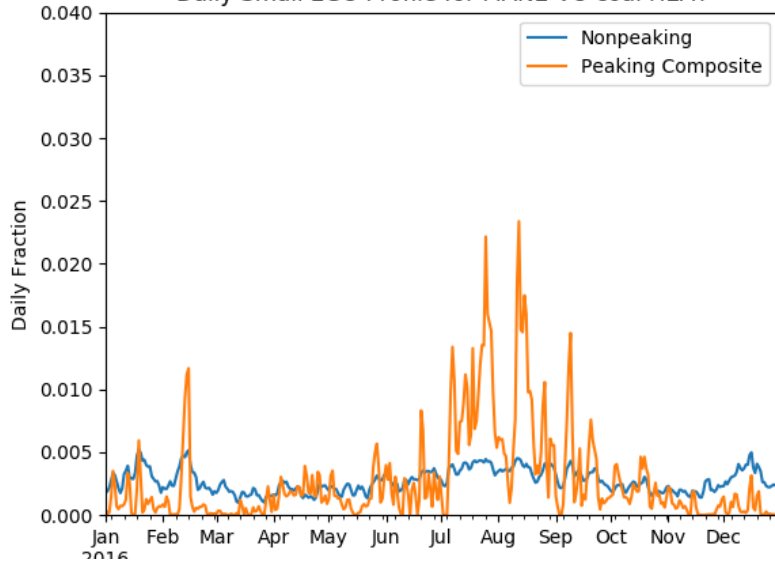
Note: the extra 24 h is for the leap day in 2016

- ▶ Unit outputs were summed from the CEMS data

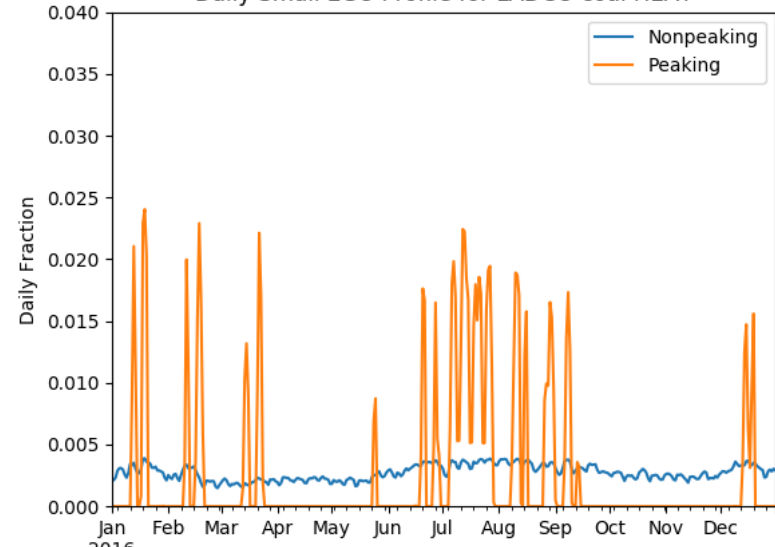
MANE-VU and LADCO Daily Profiles for Coal and Oil



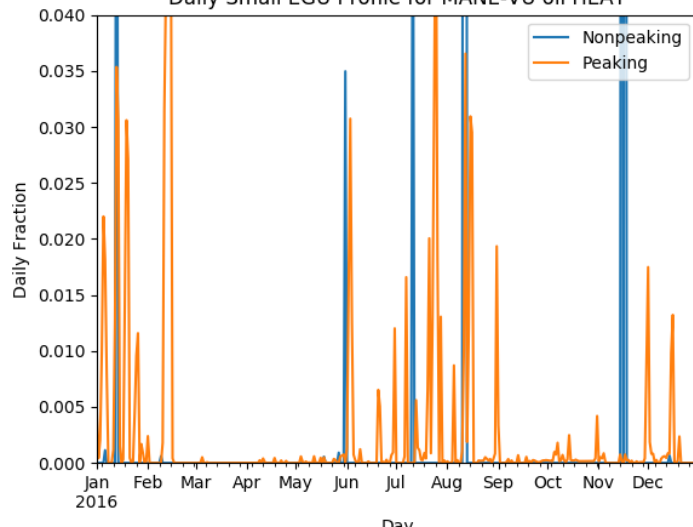
Daily Small EGU Profile for MANE-VU coal HEAT



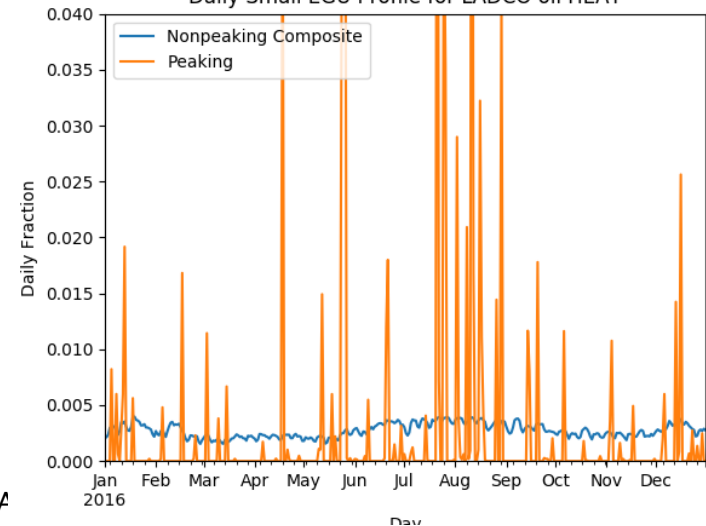
Daily Small EGU Profile for LADCO coal HEAT



Daily Small EGU Profile for MANE-VU oil HEAT



Daily Small EGU Profile for LADCO oil HEAT

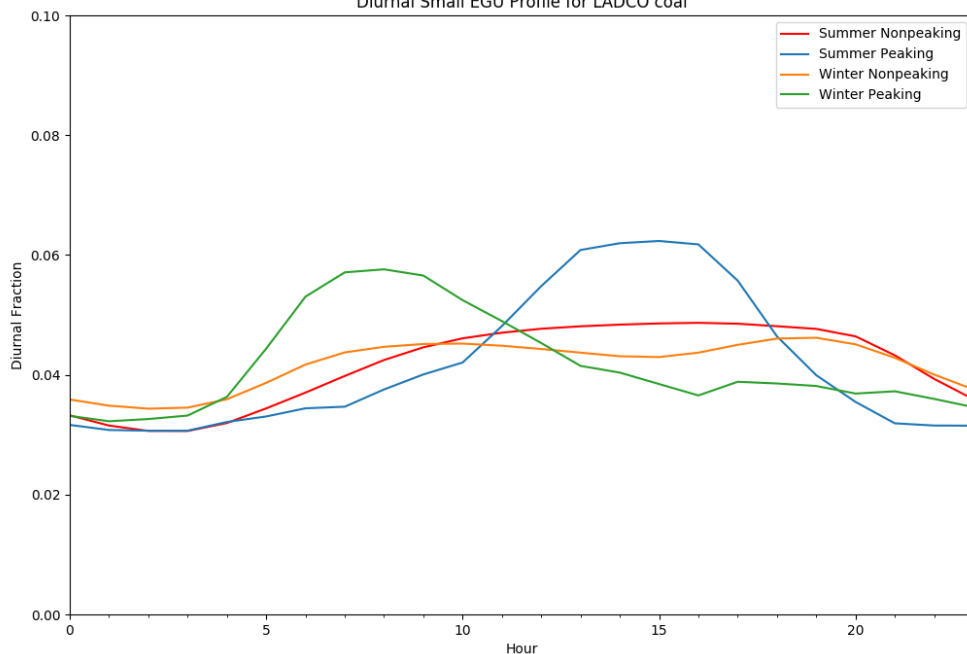




Diurnal Profiles

LADCO coal

Diurnal Small EGU Profile for LADCO coal

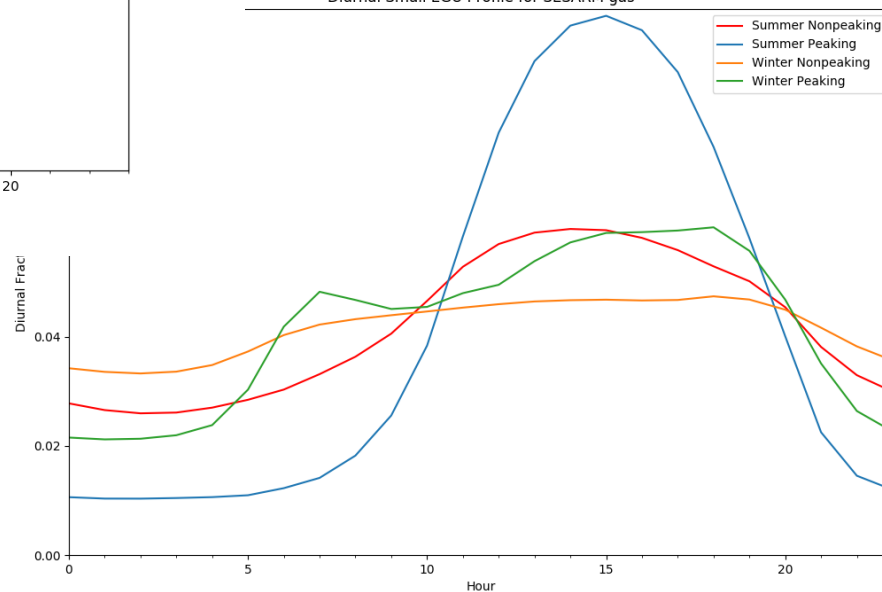


Diurnal profiles are created for each region and fuel for peaking and non-peaking

Profiles differ by region and season

SESARM gas

Diurnal Small EGU Profile for SESARM gas



Red: summer nonpeaking
Blue: summer peaking
Orange: winter nonpeaking
Green: winter peaking



QA of Temporal Allocation

- ▶ Check SMOKE Temporal logs to ensure all sources are mapped 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 (x-ref application)
- ▶ Create monthly gridded plots
- ▶ Compare daily Smkmerge reports for rwc and ag for two different Tuesdays (for example) in the same month as they should be different (except NH3_FERT) due to the Gentpro temporalization

Questions?

- ▶ Does anyone have questions on temporal allocation?



Spatial Allocation

- ▶ Spatial allocation is the process of mapping inventory emissions to modeling grid cells
- ▶ We do this using spatial surrogates; there are many types and each has a unique code (ID)
 - Population (100), Total agriculture (310), Railroad Density (261), Offshore shipping (806), Urban unrestricted daily VMT (222), Gas well count (698)
 - A cross reference maps inventory SCCs to surrogate codes

County Total Emissions

Gridded Emissions





Surrogate Tool

- ▶ Java program that takes .csv files as input
 - Runs the Spatial Allocator to prepare surrogates
- ▶ Download from <http://www.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 GIS datasets are too large to process with the Spatial Allocator (e.g., new roads, CMV)
 - NEW: PostgreSQL tool with PostGIS can also compute surrogates: <https://github.com/CMASCenter/Spatial-Allocator>

Data Used to Create a Spatial Surrogate with Surrogate Tool



- ▶ Weight Shapefile: an attribute is selected from this spatial dataset to “weight”/apportion the emissions in a county into the model grid cells
 - Population at the census tract block level (polygon)
 - 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: modeling grid cells



Spatial Surrogate values

Value =
$$\frac{\text{sum of weight attribute in grid cell}}{\text{sum of weight attribute in data polygon}}$$

Values sum to 1 for each county / province

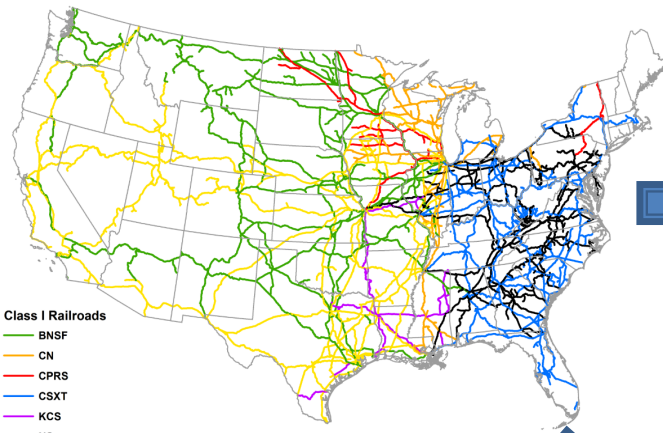
Surg ID	County	Col	Row	Ratio	Comment*
806	01003	345	207	0.2	200/1000
806	01003	346	207	0.3	300/1000
806	01003	346	208	0.5	500/1000
806	01005	355	210	0.4	800/2000
806	01005	355	209	0.6	1200/2000

* Surrogates created using the Spatial Allocator include a comment that shows how the ratio was computed

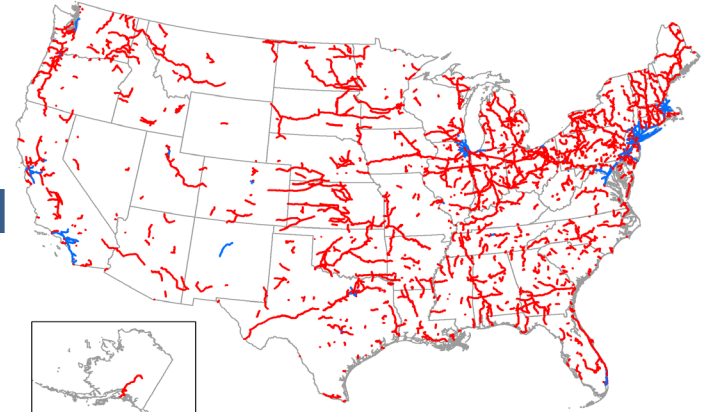
Creating a Surrogate for Railroad Miles



Weight =
Railroad miles
Data =
US. Counties
Output =
US 12km grid

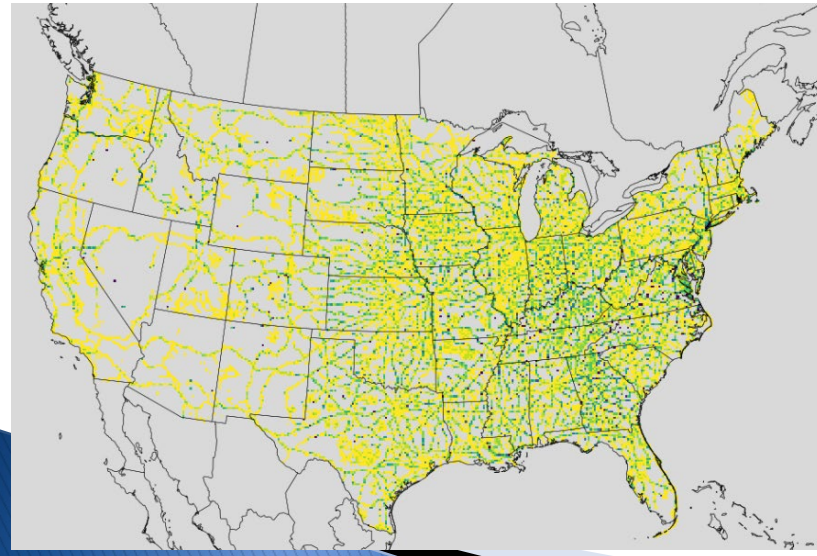


Class 2+3 Railroads

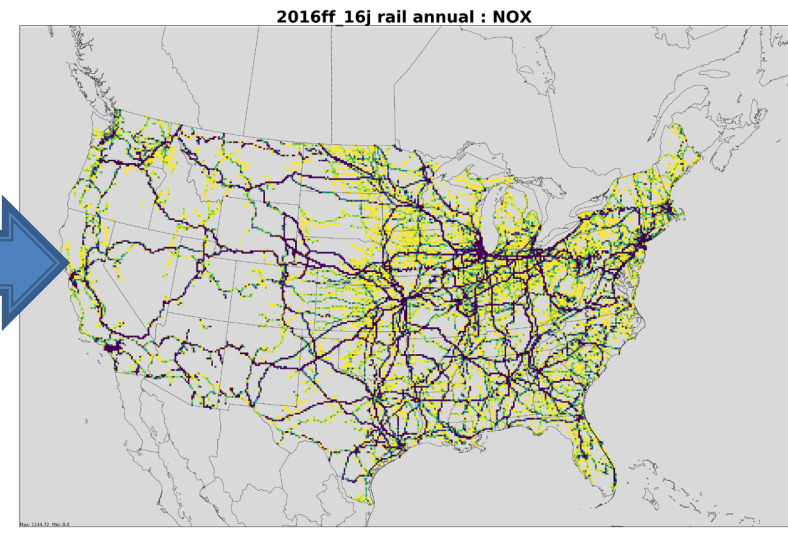
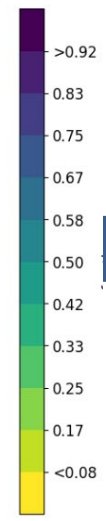


Source: Federal Railroad Administration - June 2018

Surrogate Fractions



NOx Emissions (tons/yr)



Using Cross-references and Profiles (Generically)



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

X-REF table

<u>SCC, Surg. ID</u>
2505020
2505020
2294000
2296000

Profiles table (sum to 1)

ID, Grid cell 1, 2, 3



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
008000	2520100102	689	
048243	2520100102	693	! Replaced 698
048243	2520100102	693	! Replaced 698

*A surrogate can be applied to **all counties** using code 000000 or to specific states using **state FIPS+"000"**, or to **specific counties**

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

Some Spatial Surrogate Data Sources



- ▶ National Land Cover Database (NLCD)
- ▶ U.S. Census American Community Survey
- ▶ U.S. Census Topologically Integrated Geographic Encoding and Referencing (TIGER) data
- ▶ U.S. DOT Highway Performance Monitoring System (HPMS) – Annual Average Daily Travel (AADT)
- ▶ National Transportation Atlas Database (NTAD)
- ▶ Oil and Gas Activity Data

Key Spatial Surrogates for CAPs (2014fa tons by sector)



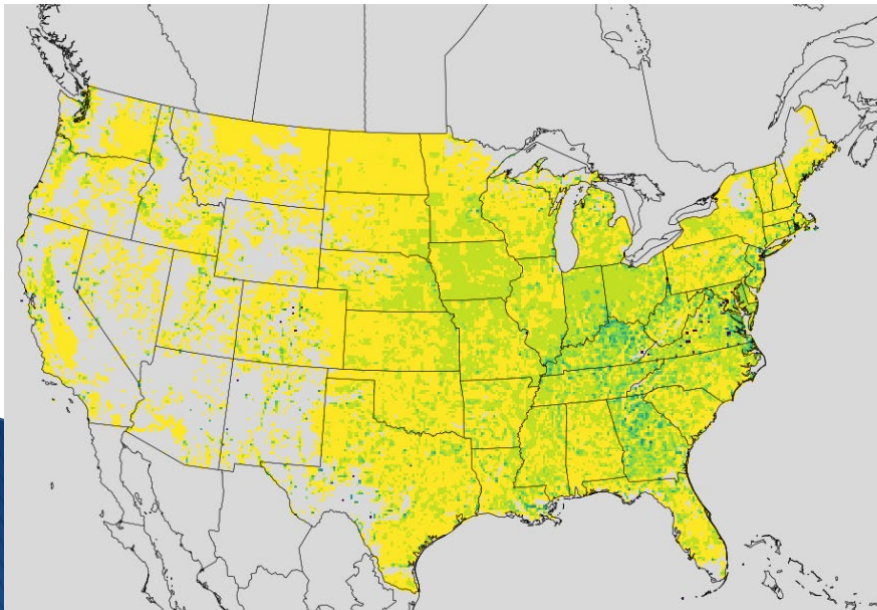
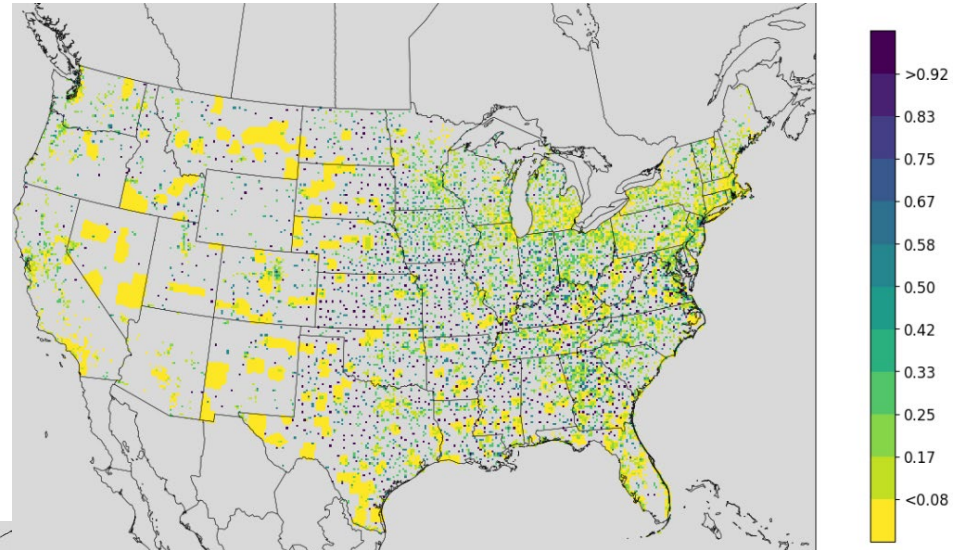
Sector	ID	Description	NH3	NOX	PM2_5	VOC
ag	310	NLCD Total Agriculture	3,135,285			
onroad	307	NLCD All Development		560,112	12,560	1,142,592
onroad	222	Urban Unrestricted AADT	42,001	1,223,593	54,345	376,209
nonpt	306	NLCD Med + High	22,268	239,863	290,187	864,662
onroad	232	Rural Unrestricted AADT	25,027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

Agriculture and Golf Course Surrogates



The golf course surrogate is based on a point Shapefile and is gapfilled* with housing (polygon surrogate)

* Gapfilling means values from another surrogate are used when the primary surrogate has no data in a county



The agriculture surrogate is based on raster data converted to polygons, gapfilled with Rural Housing

Quality Assurance of Spatial Allocation



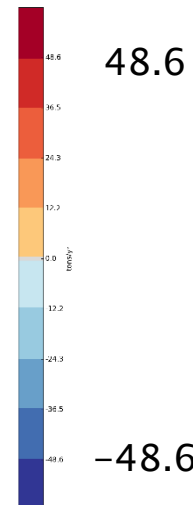
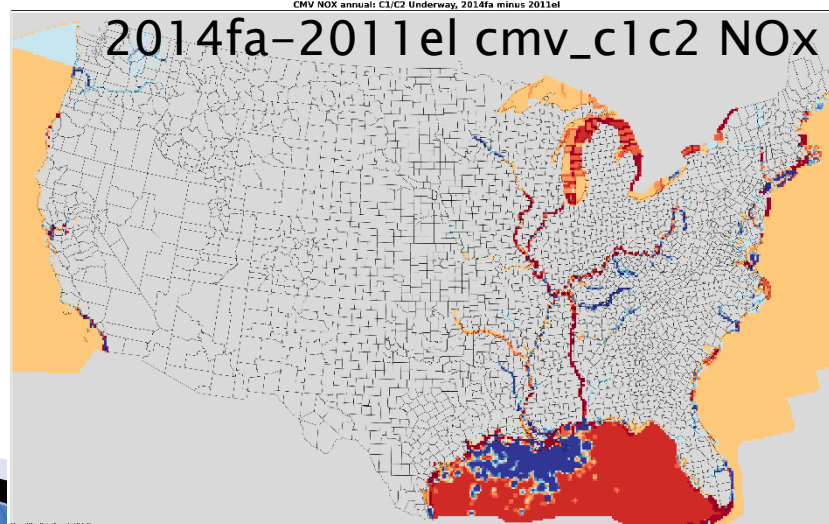
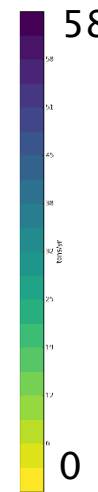
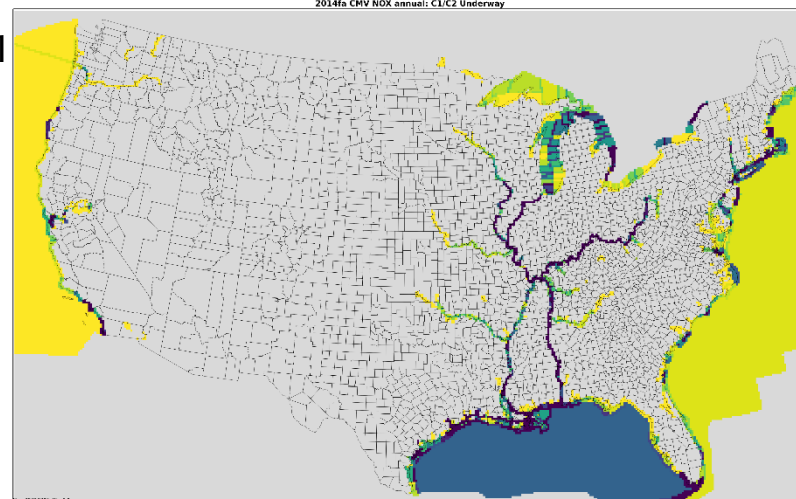
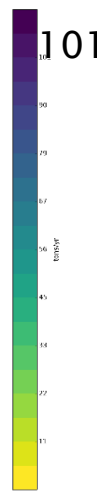
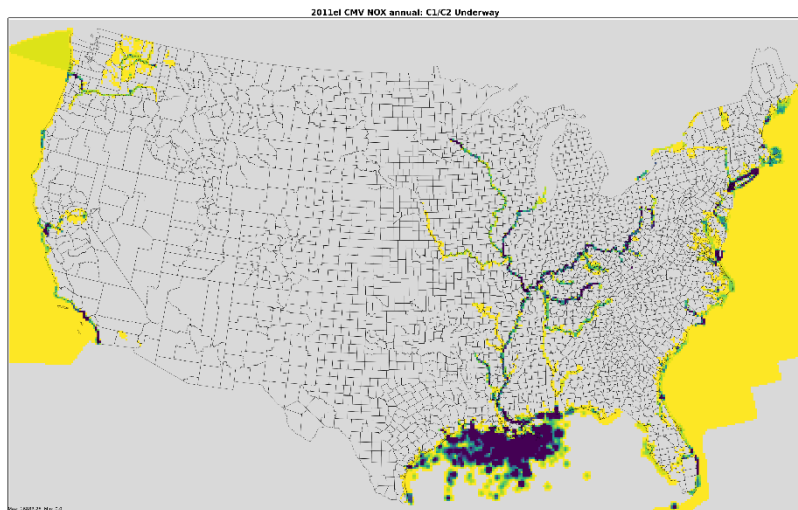
- ▶ Check SMOKE Grdmat logs to ensure all SCCs are mapped to spatial allocation profiles and only emissions outside the domain are not allocated to grid cells (do not want to drop emissions)
- ▶ Review gridded emission plots by sector to ensure spatial patterns are reasonable (US sources are all in US, onshore emissions are all on land)
- ▶ Compare post-SMOKE emissions to the inventory also helps to ensure that no emissions are dropped due to gridding
- ▶ For point sources: check that inventory coordinates fall within county boundaries

Maps Help us to QA Spatial Allocation: cmv_c1c2 Example



2011el cmv_c1c2 NOx

2014fa cmv_c1c2 NOx

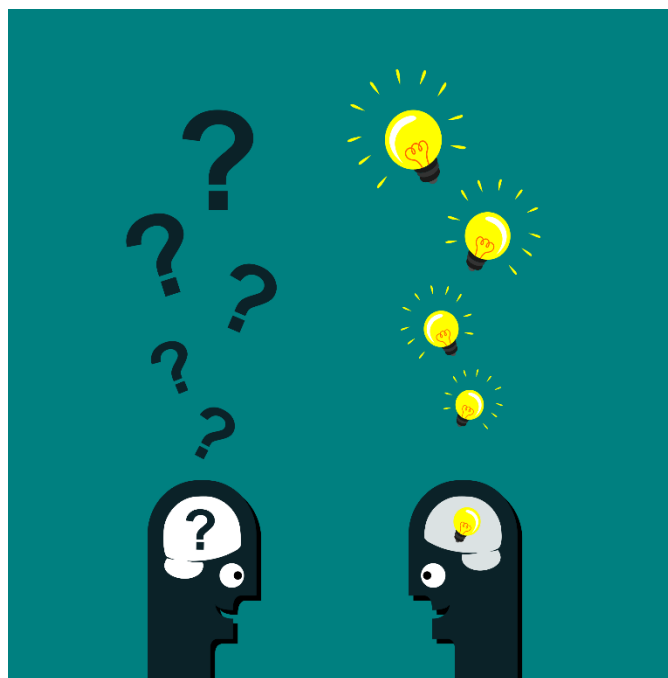


Comparing gridded emissions shows issues with surrogates

Great Lakes and Gulf of Mexico have different treatment

Questions?

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





Speciation

- ▶ Mapping inventory pollutants to model species
 - Model species are used in the air quality model (AQM)
 - NO_x, 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 sources
 - 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 5.0 is the most recent version:
<https://www.epa.gov/air-emissions-modeling/speciate>
- Includes basin-specific profiles for oil and gas sources

▶ Speciation Tool

- Processes profiles from the SPECIATE database into the chemical mechanisms used by air quality models
- Written in PostgreSQL and Perl
- Available from <http://cmasceneter.org>

Speciation Overview



Inventory Poll

Profile (%)

Model species 1

Model species 2

Model species 3

Model species 4

Speciated (mass)

Model species 1

Model species 2

Model species 3

Model species 4

MW1

MW2

MW3

MW4

Conversion to moles



NO_x Speciation

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

profile	pollutant	species	massfrac
WHONO	NOX	NO ₂	0.092
WHONO	NOX	NO	0.900
WHONO	NOX	HONO	0.008
NHONO	NOX	NO ₂	0.100
NHONO	NOX	NO	0.900



PM_{2.5} Speciation

- ▶ Older versions of CMAQ used “simplified” PM model species (AE5)
- ▶ Recent versions of CMAQ use 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: $\text{VOC} * 1.199 = \text{TOG}$ (also includes methane)
- ▶ TOG is then speciated according to the mechanism (species sum to 1.0):
 - Different model species depending on the chemical mechanism (e.g., CB05, CB6)

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 (8751 a)

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 Overview

▶ Integration

- Process of taking select VOC HAPs from the inventory as “true” and then speciating the remaining VOC
- Want to avoid double counting of pollutants
- Want to speciate the remaining VOC, while taking into account HAPs that were removed

▶ NBAFM taken from inventory as “explicit HAPs”

- Naphthalene, Benzene, Acetaldehyde, Formaldehyde, Methanol

▶ NONHAPTOG

- Remaining TOG after removing explicit VOC HAPs
- $\text{NONHAPTOG} = \text{TOG} - \text{Total of NBAFM species}$



VOC Integration Example

Gasoline Exhaust – E10 (8751a)

No integrate (CB05)

Integrate (CB05)

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

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 by Sector

Platform Sector	Approach for integrating in 2016ff
ptegu	No integration (i.e., integrated species in inventory ignored)
ptnonipm	No integration
pt_oilgas	No integration
ptfire, ptagfire	Partial integration
ptfire_othna	No integration
othar	No integration
othpt	No integration
onroad_can	No integration
onroad_mex	Full integration (MOVES-Mexico)
ag	Partial integration
afdust, othafdust, othptdust	N/A - sectors contain no VOC
beis	N/A - contains specific VOC model species
nonpt	Partial integration (NBAFM)
np_oilgas	Partial integration (NBAFM)
rwc	Partial integration (NBAFM)
rail	Full integration (NBAFM)
nonroad	Full integration (calculated in MOVES2014b)
cmv_c1c2	Full integration (NBAFM)
cmv_c3	Full integration (NBAFM)
onroad	Full integration (calculated in the MOVES2014 model)



Onroad speciation

- ▶ MOVES2014b 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 (as 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 Spcmat SMOKE logs to ensure that all sources have references to VOC and PM speciation profiles.
- ▶ Sum model species to compare to VOC and PM_{2.5} 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:
 - NBAFM but no VOC for an integrate source
 - No TOG conversion factor
 - Skipping pollutant [X] for other than PM₁₀ 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?

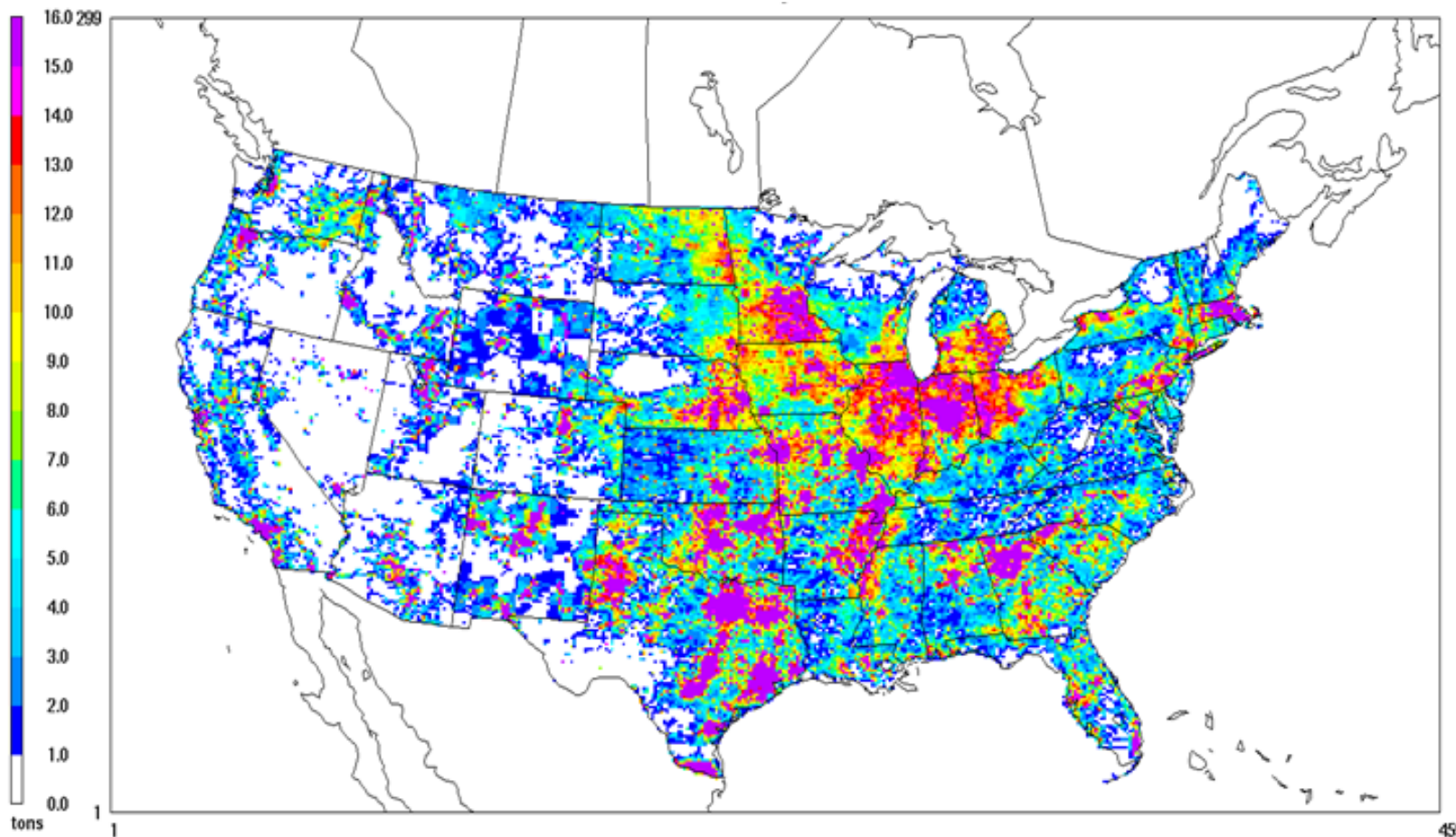




Area Fugitive Dust Adjustments

- ▶ AQ models tend to overestimate the impact of fugitive dust emissions
 - Paved and unpaved roads, construction, mining, hooves
- ▶ Prior to modeling, afdust 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

Unadjusted Fugitive Dust $PM_{2.5}$ Emissions



▶ Note: in NEI, dust emissions are adjusted

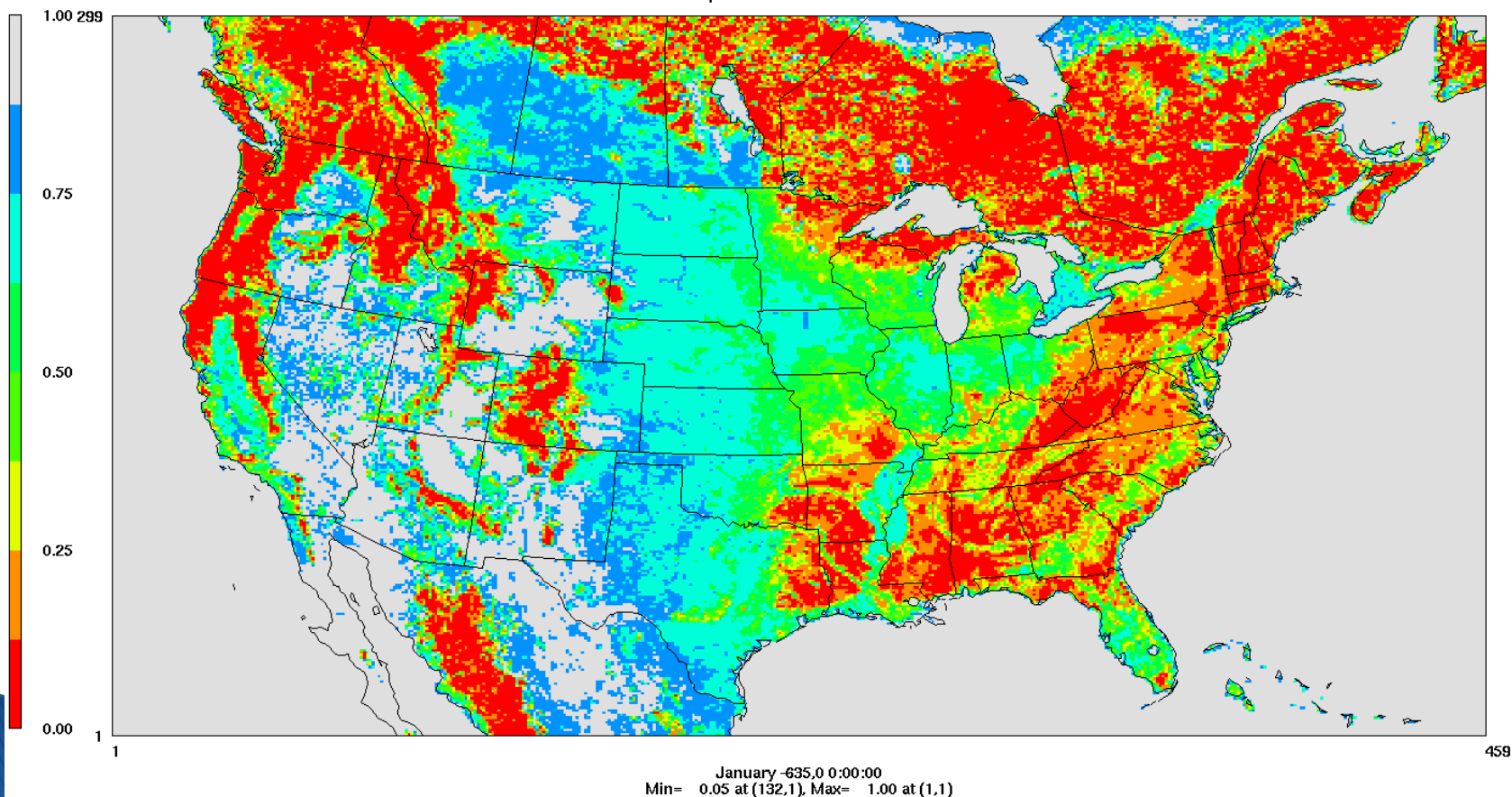


Transport Fraction Plot

Red = high level of reduction; Gray = little reduction

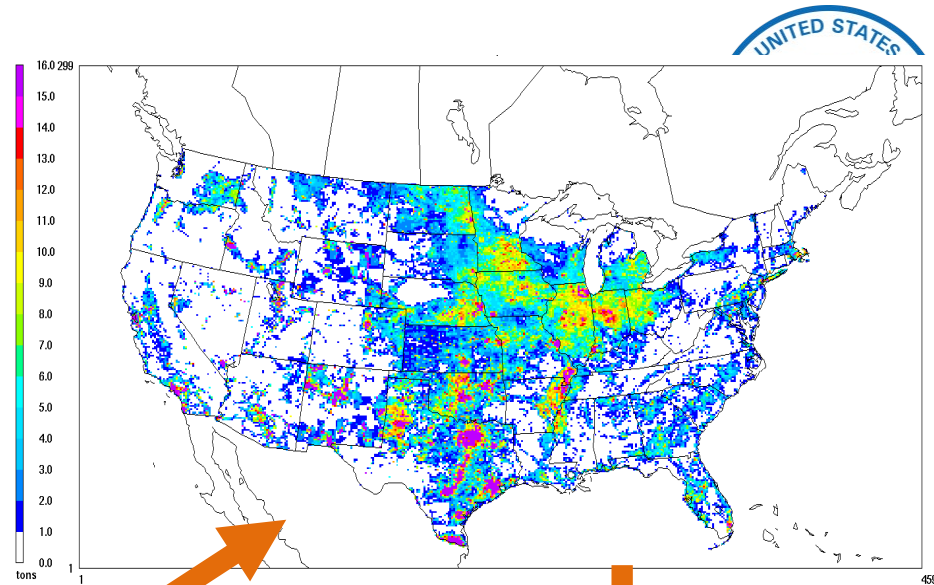
Layer 1 xportfrac

a=xportfrac.12US1.from4km.ncf



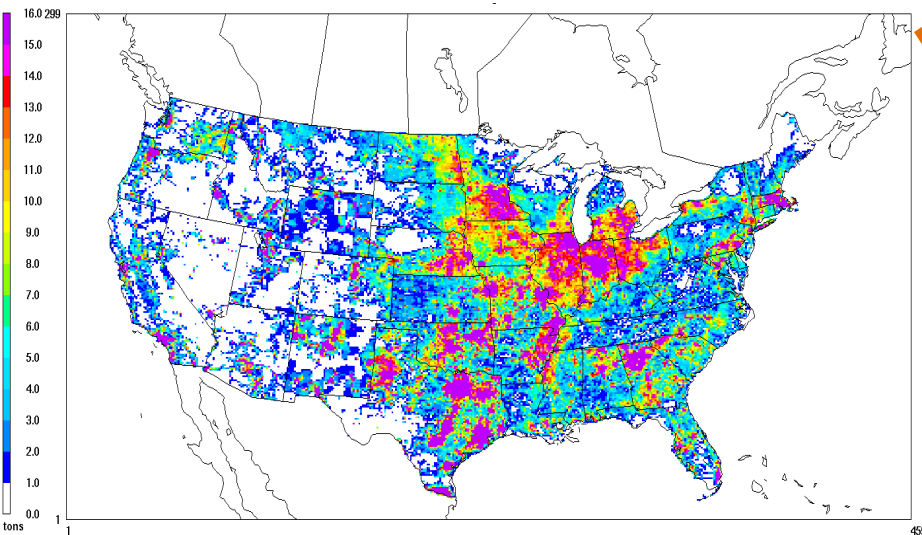
Impact of afdust Adjustments

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

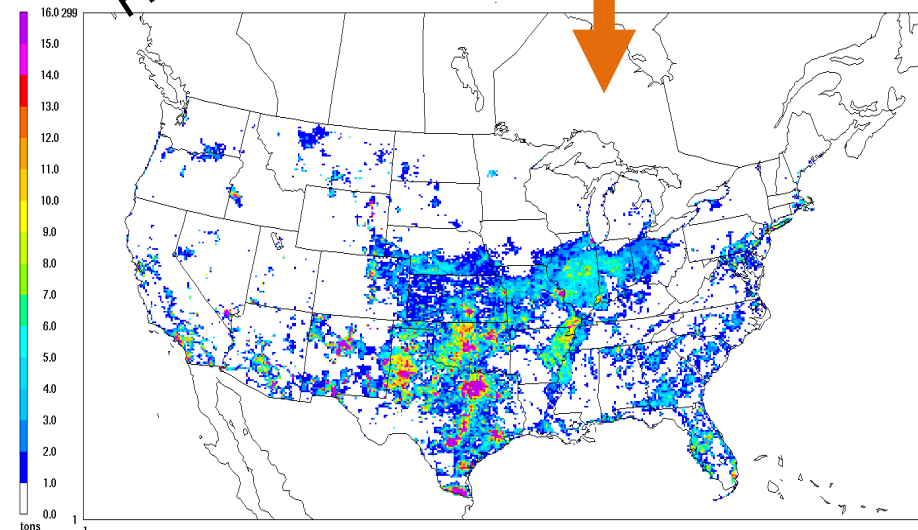


Apply Transport Fraction

Precipitation adjustment



Unadjusted emissions



BEIS 3.6.1: Updated Biogenic Emissions



- ▶ Updated leaf temperature algorithm in v3.6.1
 - Leaf temperature calculated using canopy model rather than 2 meter temperature
- ▶ Biogenic Emissions Landcover Database (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 3.6.1



Variable	Description
LAI	leaf-area index
PRSFC	surface pressure
Q2	mixing ratio at 2 m
RC	convective precipitation per met TSTEP
RGRND	solar radiation reaching surface
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



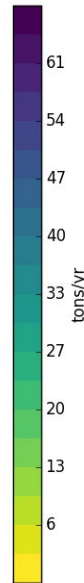
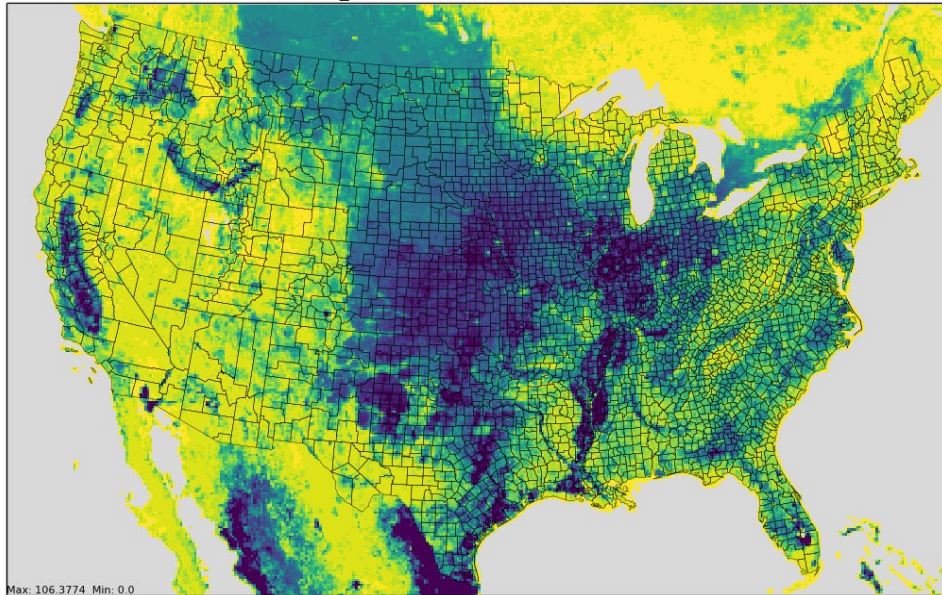
Species Produced by BEIS

- ▶ 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

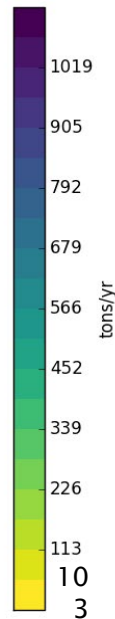
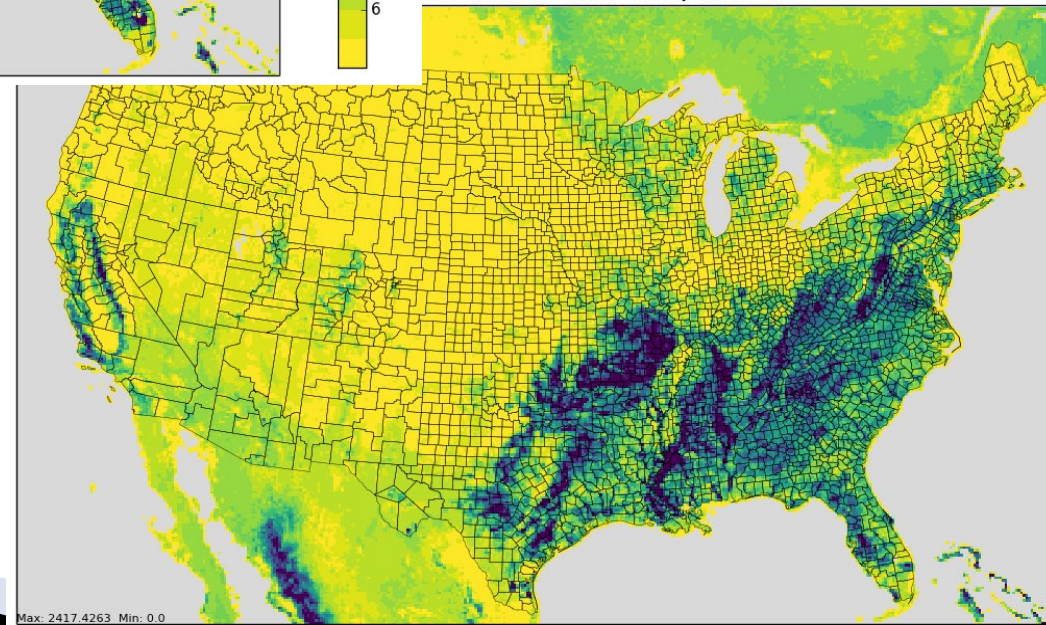


2014fa_nata beis NO emissions, annual



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

2014fa_nata beis ISOP emissions, annual



▶ Bottom: Isoprene (produced during photosynthesis)

Future Directions and Questions?



- ▶ Continue examining alternative biogenic model Model of Emissions of Gases and Aerosols from Nature (MEGAN) version 3 biogenic emissions estimates
 - MEGAN used for global and hemispheric modeling and for regional modeling by some agencies
- ▶ Continue examining new Canadian BELD4-compatible data
- ▶ Updated BELD(5?) coming soon
- ▶ Any questions on fugitive dust or biogenic emissions?



NEI Fire Inventory Details

- ▶ Includes daily “point” emissions from wildfires and prescribed fires
- ▶ Emissions were estimated for $PM_{2.5}$, PM_{10} , CO, CO_2 , CH_4 , NO_x , NH_3 , SO_2 , VOC, and 34 hazardous air pollutants (HAPs). $PM_{2.5}$ emissions were further broken down into EC, OC, SO_4 , NO_3 , and PM fine
- ▶ HAPs emission factors and fractions of $PM_{2.5}$ components were provided by EPA
- ▶ 2014 NEI made flaming and smoldering emissions available (to allow for differentiated treatment of plume rise and potentially speciation)
- ▶ Fire Inventory from NCAR (FINN) is used for Puerto Rico



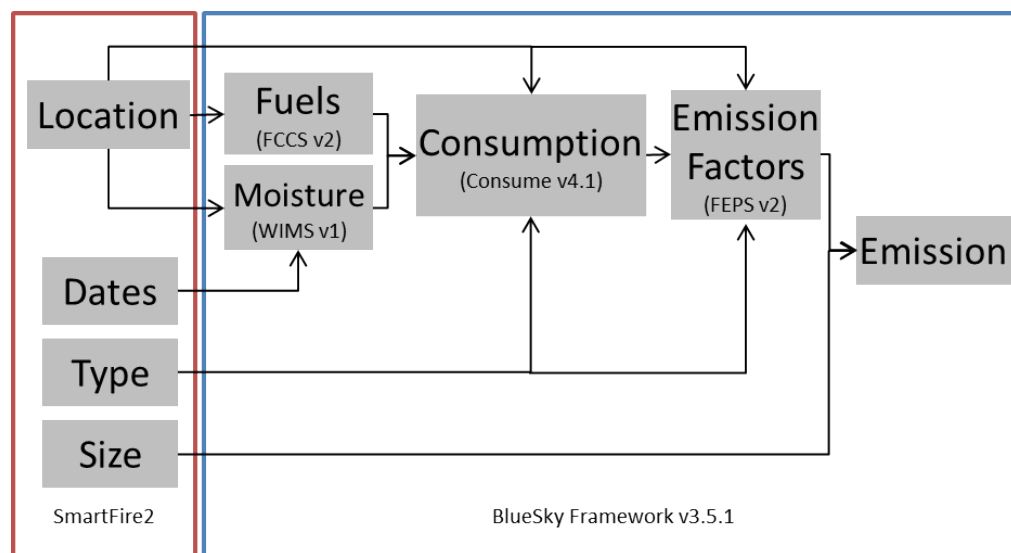
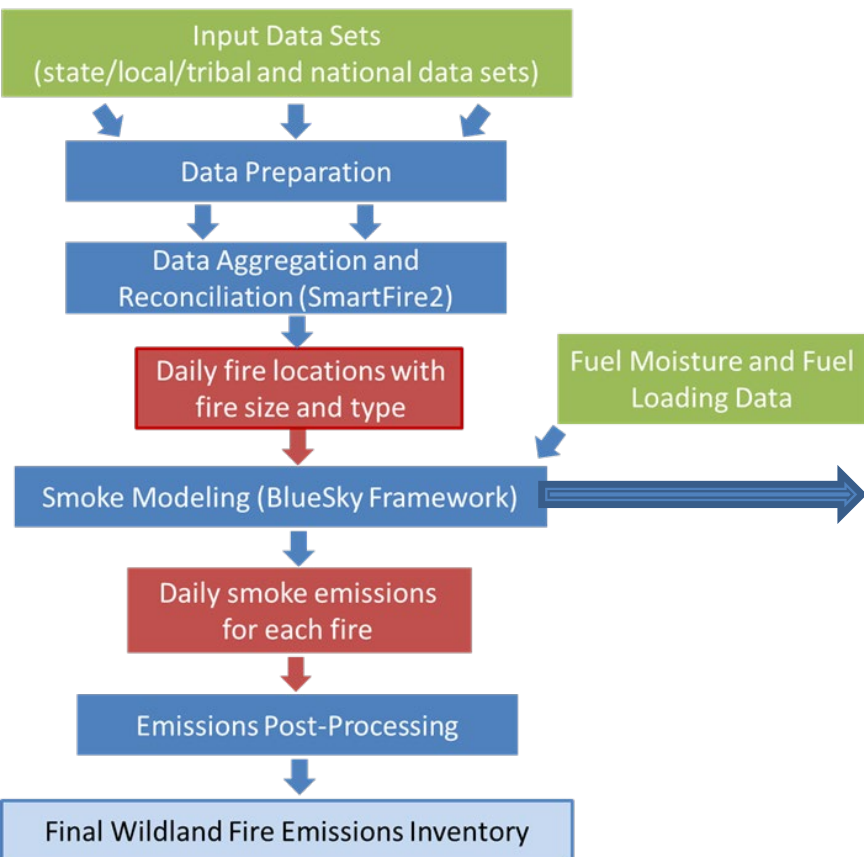
Data Sources for NEI Fires

- ▶ Data Sources included for NEI fire inventory development (non-NEI years typically use only data in red)
 - State/local/tribal data
 - National Association of State Foresters (NASF) WF data
 - NOAA's Hazard Mapping System (HMS) data
 - Incident Status Summary (ICS-209) data (wild vs prescribed)
 - Geospatial Multi-Agency Coordination (GeoMAC) fire perimeter Shapefiles
 - Monitoring Trends in Burn Severity (MTBS)
 - USDA Forest Service Activity Tracking System (FACTS) Rx fire perimeter data
 - U.S. Fish and Wildlife Service (USFWS) data
 - U.S. Department of Interior (DOI) Rx data

- ▶ Ancillary data sources
 - Fuel moisture data from the USFS Weather Information Management System
 - Fuel Characteristic Classification System (FCCS) fuel loading database



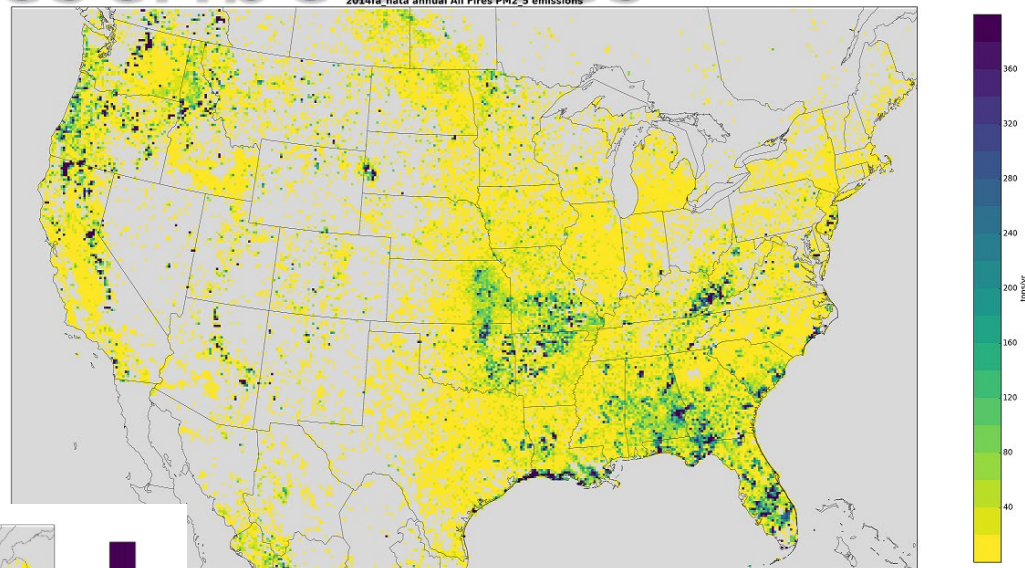
NEI Fire Development Overview



2014 and 2016 Annual PM2.5 from Wild and Prescribed Fires

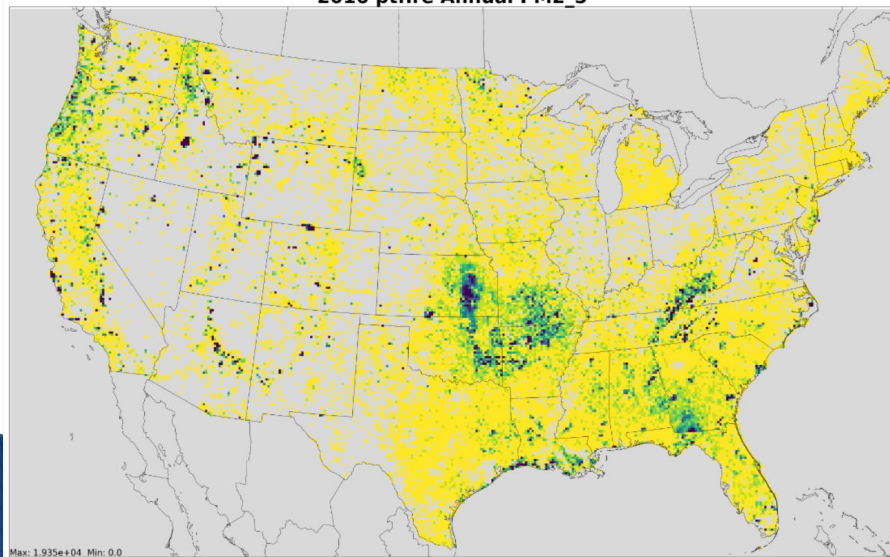


Top: 2014



Bottom: 2016

2016 ptfire Annual PM2_5



Some aspects of fires are similar between years:
Prairie, gulf coast, South Florida

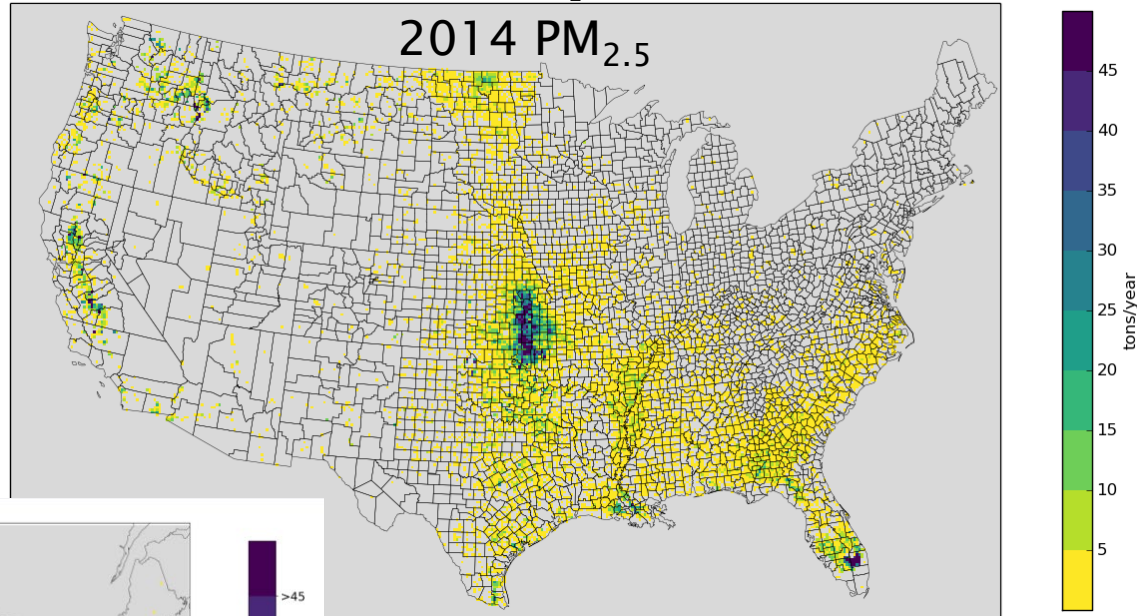
Locations of large fires vary – particularly noticeable in West, MN

Agricultural Fires

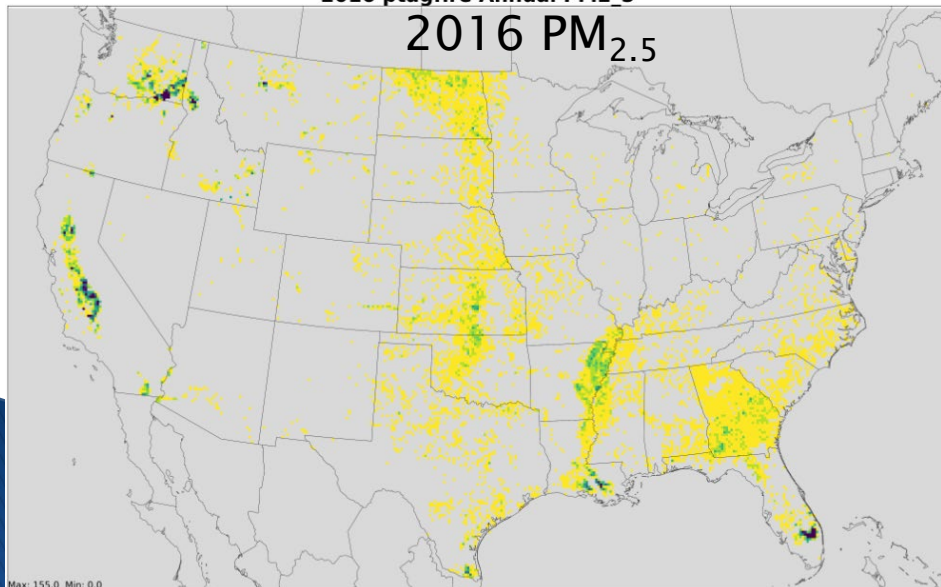


EPA estimates day-specific point-based agricultural fires based on satellite detects (Pouliot, 2017)

Point Agricultural Fires PM_{2.5} - Annual 2014



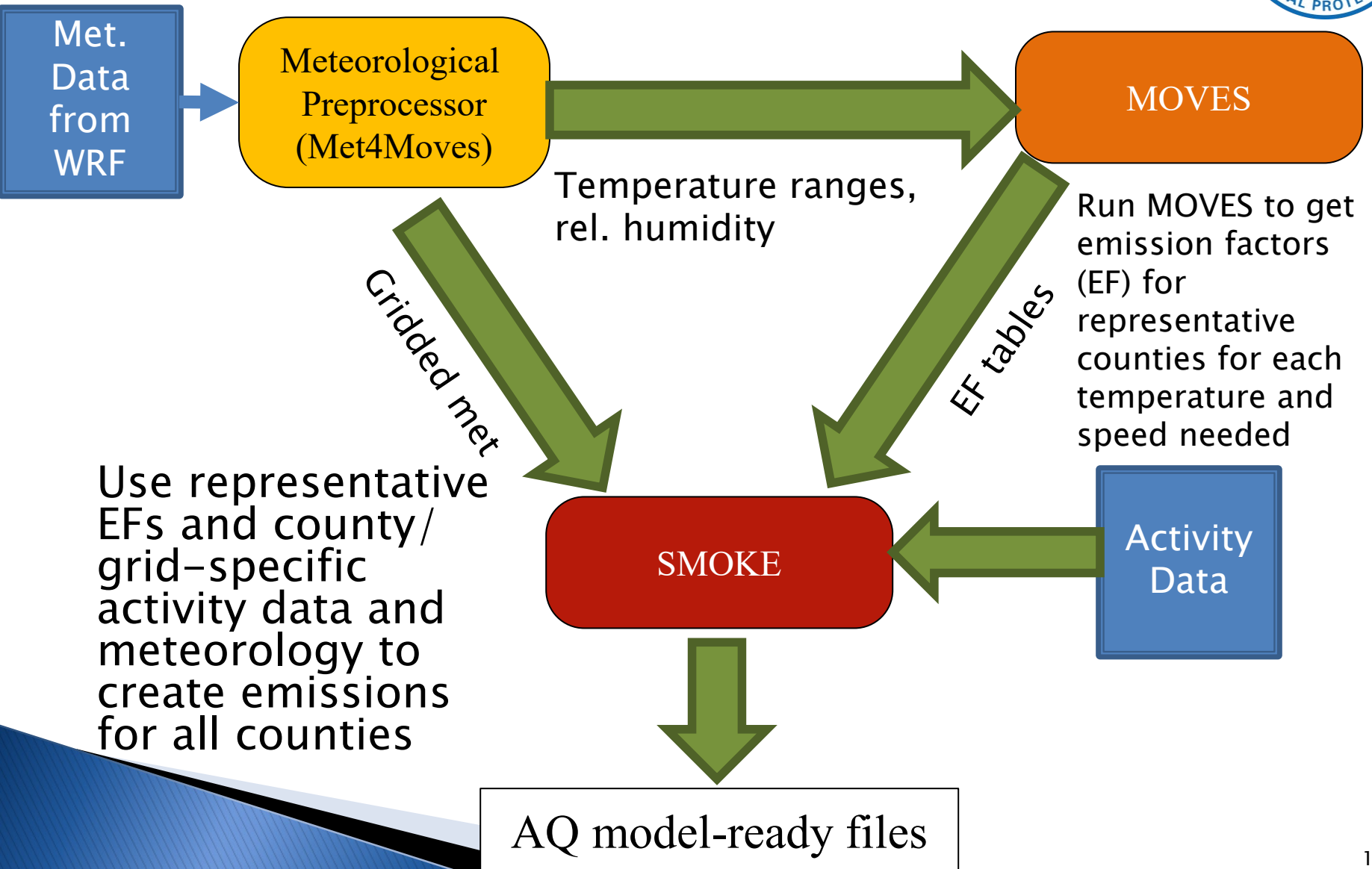
2016 ptagfire Annual PM_{2.5}



Questions?



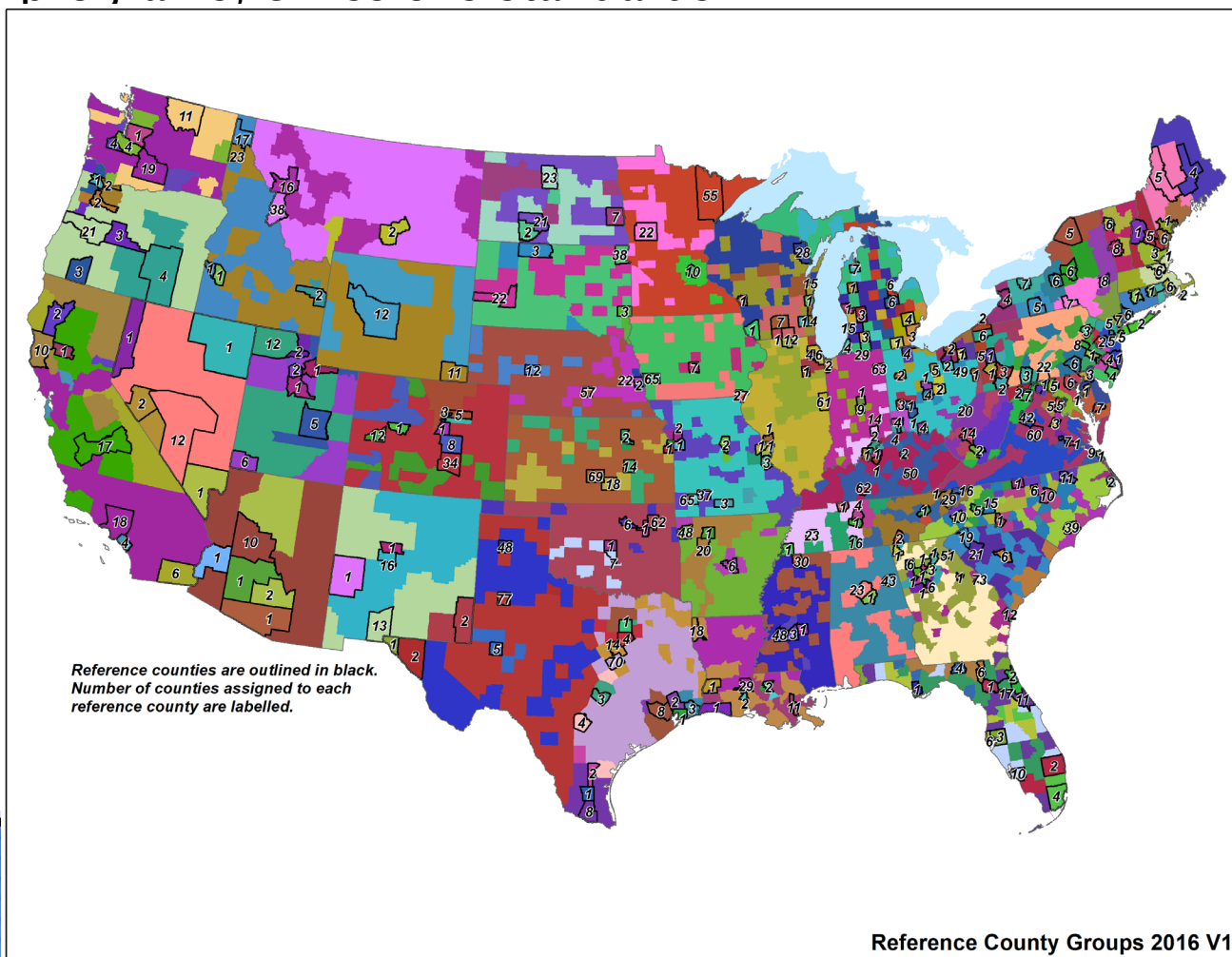
Onroad Emissions Modeling





Representative Counties

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





Onroad Emission Processes and Inputs

- ▶ On-roadway emissions
 - Exhaust, evaporative, evaporative permeation, refueling, brake and tire wear (Rate-per-distance)
 - *Primary inputs:* vehicle miles traveled (VMT), average speeds, speed profiles, and temperature (gridded, hourly)
- ▶ Off-network emissions (i.e. parked vehicles)
 - Exhaust from starts, evaporative, evaporative permeation, refueling, hot soak (right after a trip) (Rate-per-vehicle)
 - Evaporative fuel vapor venting and diurnal (when vehicles are parked for a long period) (Rate-per-profile)
 - *Primary inputs:* vehicle population (VPOP) and Temperature (gridded, hourly, daily min/max)
- ▶ Hoteling:
 - Extended idle and auxiliary power units (APU) for combination long-haul trucks (Rate-per-hour)
 - *Primary inputs:* Hoteling hours and Temp. (gridded, hourly)

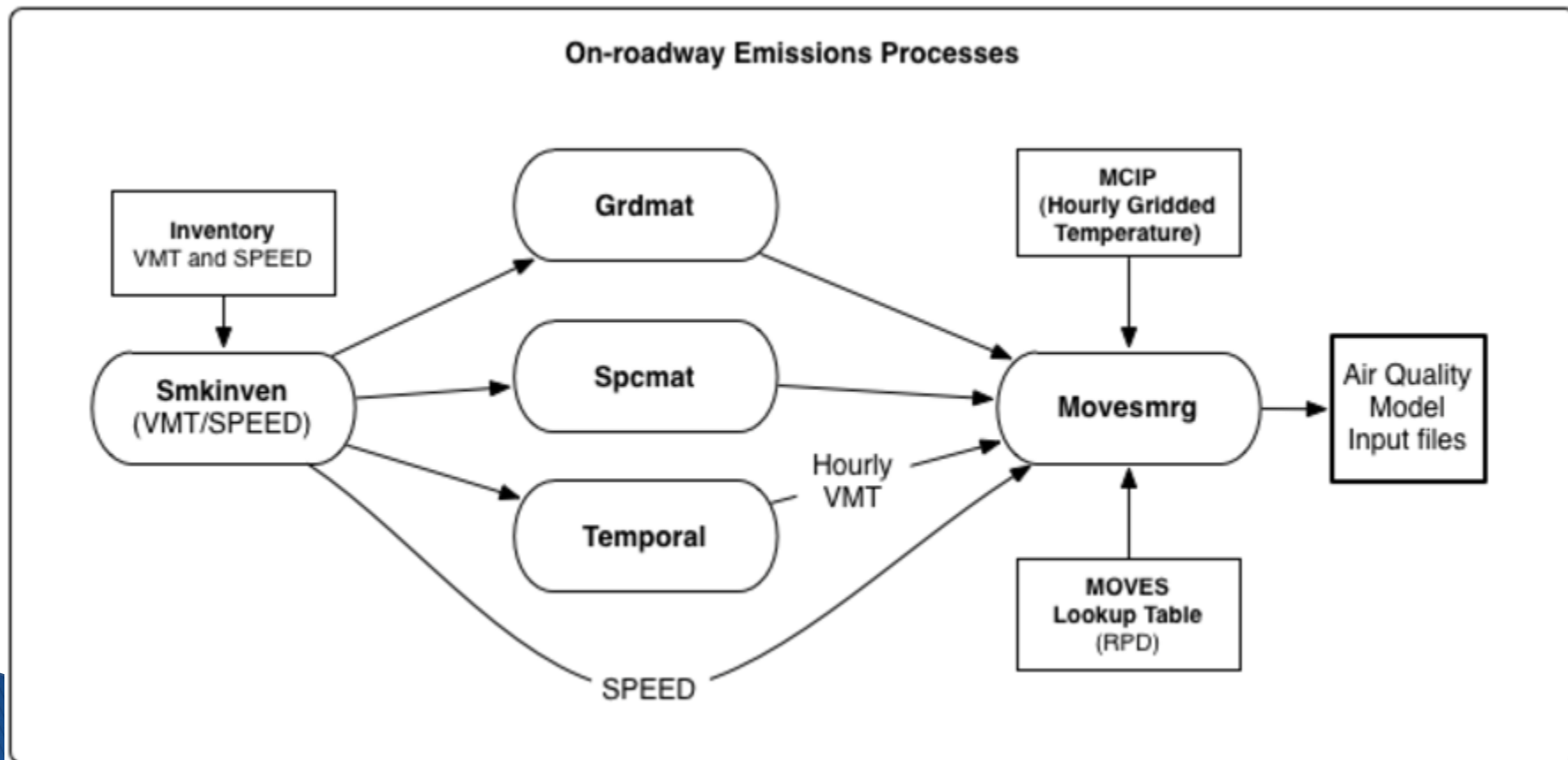


Running MOVES

- ▶ MOVES runs on Windows, but SMOKE runs on Linux so a translation step is required
- ▶ For info on running MOVES to create emission factors for SMOKE–MOVES see:
<https://github.com/CEMPD/SMOKE–MOVES>
- ▶ `runspecgenerator.pl` creates MOVES configuration files
- ▶ `moves2smkEF.pl` reads the MOVES output databases and converts them into a form that runs SMOKE

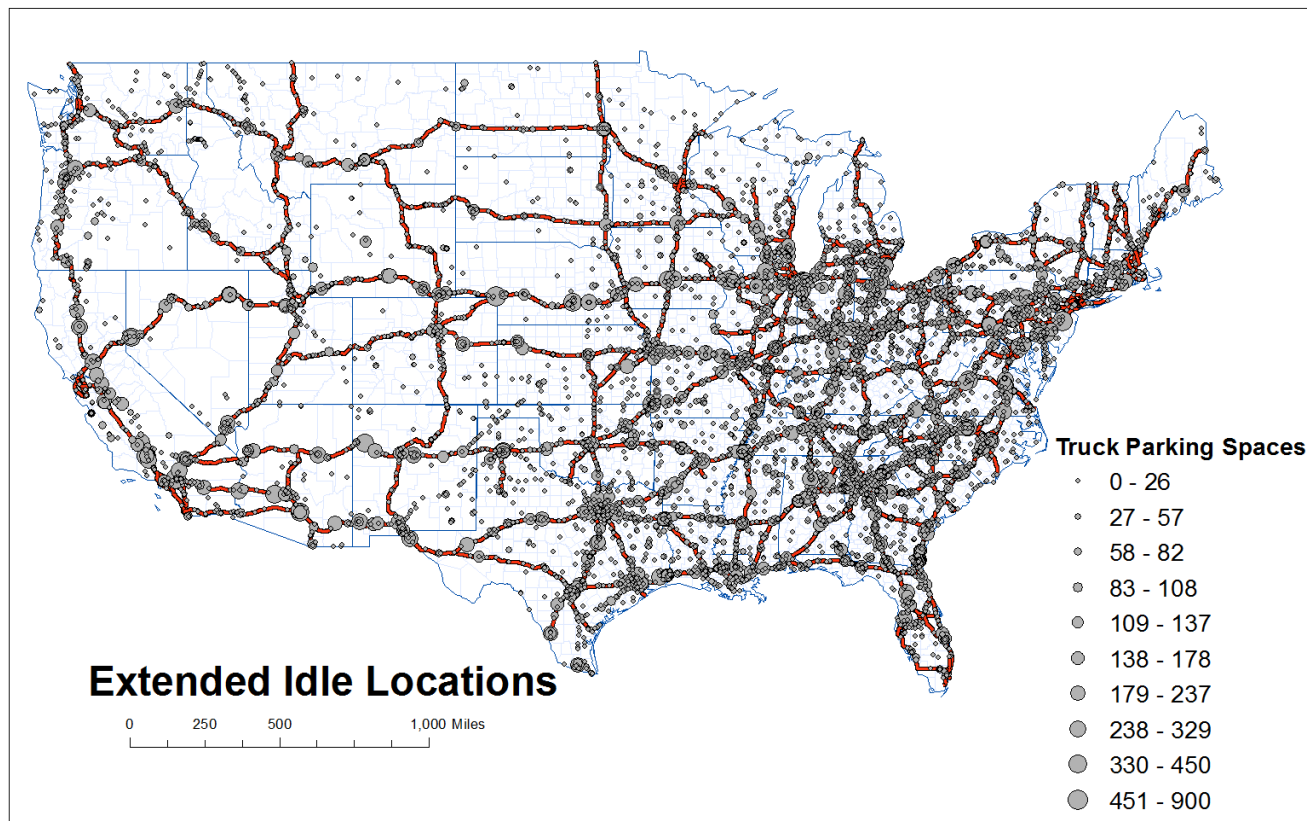
On-roadway Processing (RPD)

- ▶ Uses Standard SMOKE programs + Movesmrg
 - Input “inventory” is VMT and SPEED data



Onroad Hoteling

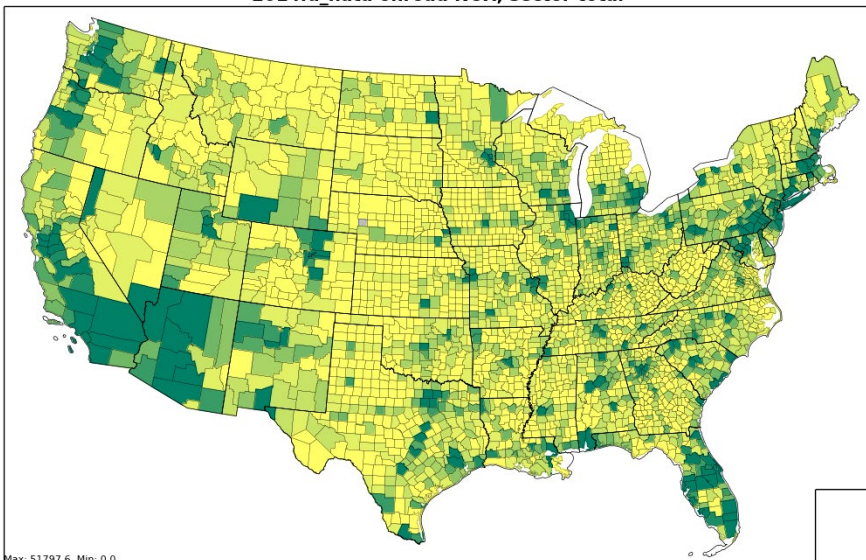
- ▶ Hoteling = Overnight truck idling: extended idle and APU
- ▶ States can submit hoteling hours by county
- ▶ EPA uses combination long-haul truck VMT on urban + rural restricted roads to distribute hoteling hours to counties
- ▶ Temporal profile is opposite of the driving profile
- ▶ Spatial surrogate is based on truck parking spaces



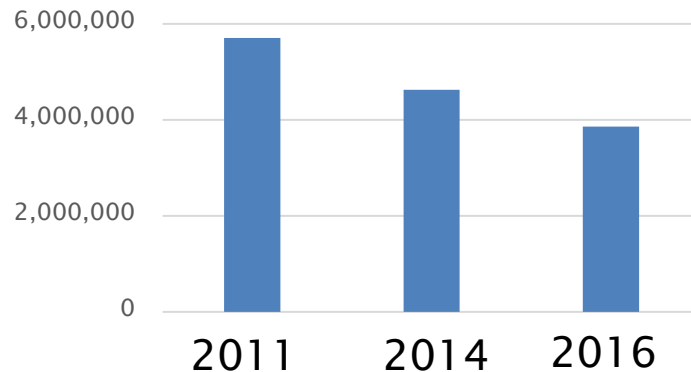
Onroad NOx Changes 2011–2014



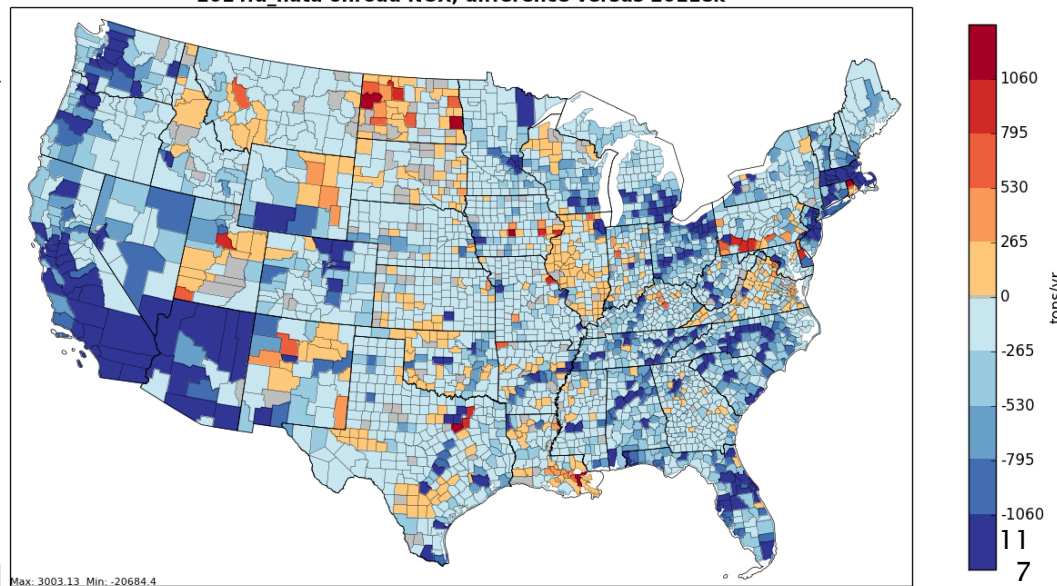
2014fa_nata onroad NOx, sector total



Onroad NOx Trend



2014fa_nata onroad NOx, difference versus 2011ek



Although VMT typically increases with time, emissions decrease as newer cleaner vehicles penetrate the market

Max: 3003.13 Min: -20684.4

Improved MOVES Inputs used in 2016



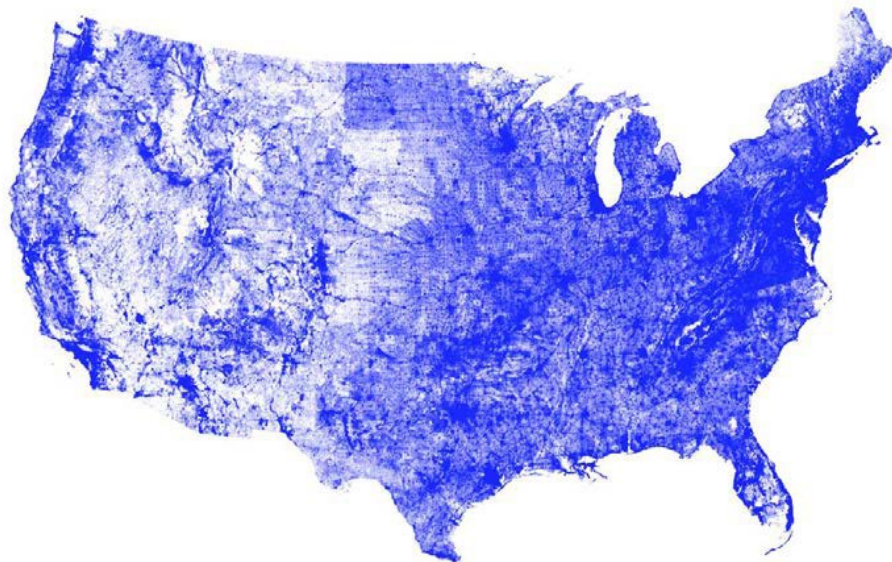
- ▶ States provided inputs for the 2016 platform
 - Activity data, other MOVES inputs
- ▶ Coordinating Research Council (CRC) sponsored a project to decode year 2017 registration VINs into MOVES vehicle types by model year for both light-duty and heavy-duty vehicles
 - Impacts age distributions and vehicle populations
 - Includes data for populations of alternative fuel light-duty vehicles (i.e., diesel, CNG, E-85, electric)
 - EPA derived VMT data based on the new VPOP data

Input Data Updates from the CRC A-100 Study



- ▶ Sponsored by the Coordinating Research Council (CRC)
- ▶ Main data source: StreetLight Data, Inc.
 - 5 Billion observations over continental U.S.
 - Passenger cars, commercial truck fleet management systems
 - Sub-minute level data for 12 consecutive months
 - Grouped by light-duty (LD), medium-duty (MD), and heavy-duty (HD); no car/truck split or age info available for LD vehicles
 - 5m spatial precision, 16 speed bins
- ▶ Used data to derive
 - VMT temporal distributions for MOVES and SMOKE temporal profiles
 - Road type distributions supplemental to those from FHWA
 - Speed distributions for MOVES plus speed inputs to SMOKE
 - Populating all speed bins by road type, month, day, hour, vehicle type was a challenge outside of urban areas

CRC A-100 Geographic Scale



18,644,352 road segments over the Continental U.S.



3,601 polygons of urban areas / clusters from the U.S. Census

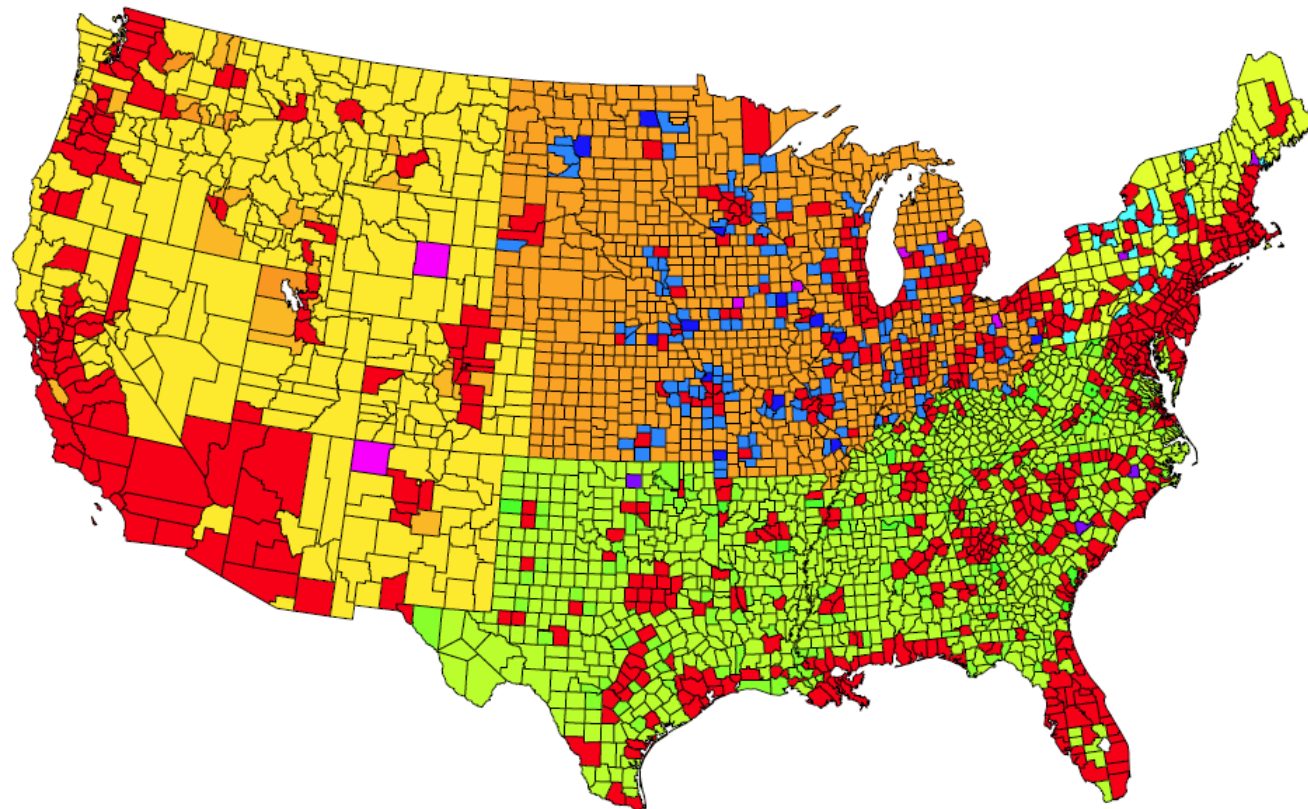
* CRC A-100 plots courtesy ERG

Spatial Groups Used



Example of Passenger Vehicles on Urban Unrestricted Roads

Counties for which MOVES inputs could be populated shown in red; others are based on data for the region and urban/rural

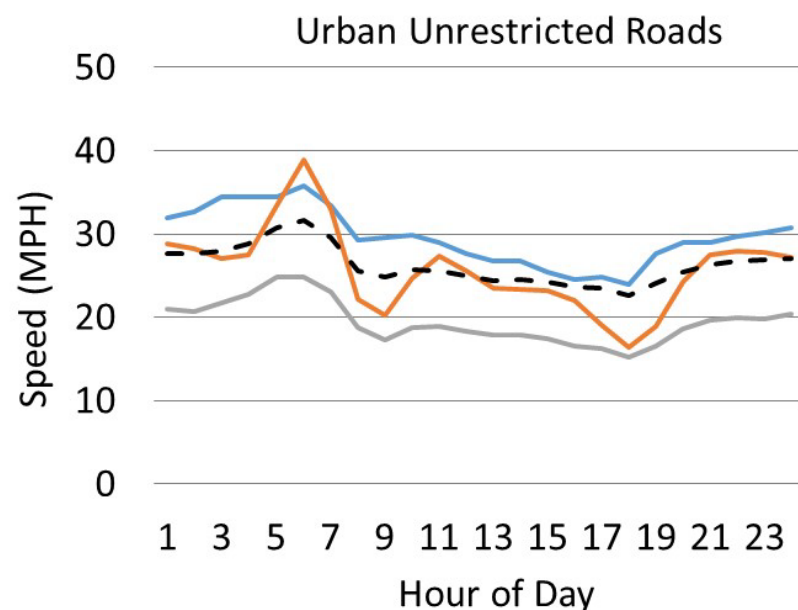
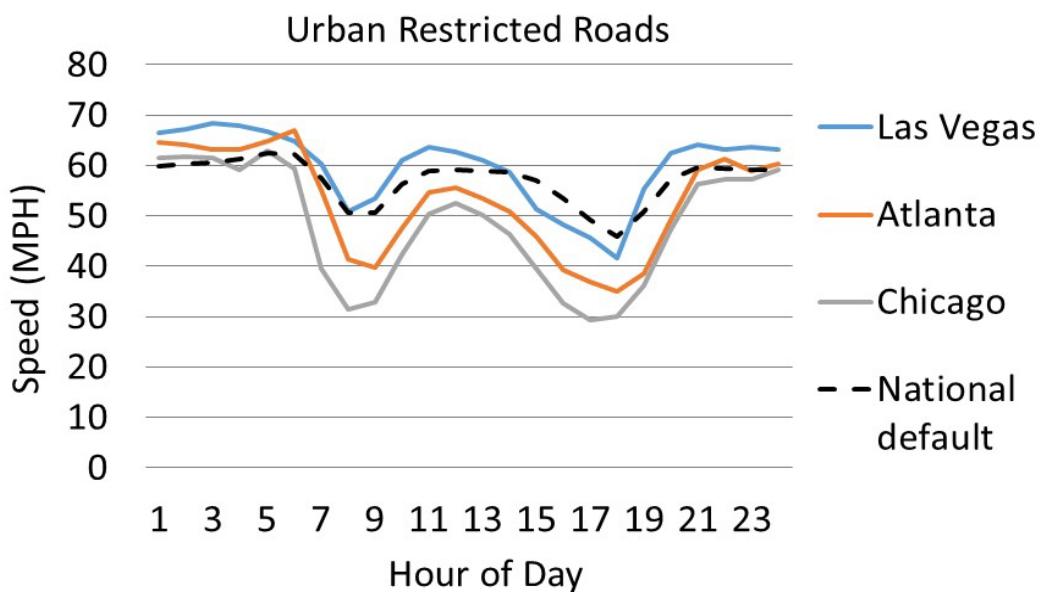


Group	Color	Description
Individual	Red	Individual
Midwest Region Average of Single County MSA Counties	Purple	Midwest Region Average of Single County MSA Counties
Midwest Region non-MSA Average	Orange	Midwest Region non-MSA Average
Northeast Region Average of Single County MSA Counties	Light Purple	Northeast Region Average of Single County MSA Counties
Northeast Region non-MSA Average	Light Orange	Northeast Region non-MSA Average
South Region Average of Single County MSA Counties	Light Purple	South Region Average of Single County MSA Counties
South Region non-MSA Average	Light Orange	South Region non-MSA Average
West Region Average of Single County MSA Counties	Purple	West Region Average of Single County MSA Counties
West Region non-MSA Average	Orange	West Region non-MSA Average
Midwest Region Average of Core Counties inside MSAs	Dark Blue	Midwest Region Average of Core Counties inside MSAs
Midwest Region Average of non-Core Counties inside MSAs	Light Blue	Midwest Region Average of non-Core Counties inside MSAs
Northeast Region Average of Core Counties inside MSAs	Dark Blue	Northeast Region Average of Core Counties inside MSAs
Northeast Region Average of non-Core Counties inside MSAs	Light Blue	Northeast Region Average of non-Core Counties inside MSAs
South Region Average of Core Counties inside MSAs	Dark Blue	South Region Average of Core Counties inside MSAs
South Region Average of non-Core Counties inside MSAs	Light Blue	South Region Average of non-Core Counties inside MSAs
West Region Average of Core Counties inside MSAs	Dark Blue	West Region Average of Core Counties inside MSAs
West Region Average of non-Core Counties inside MSAs	Light Blue	West Region Average of non-Core Counties inside MSAs



Speed Results by City

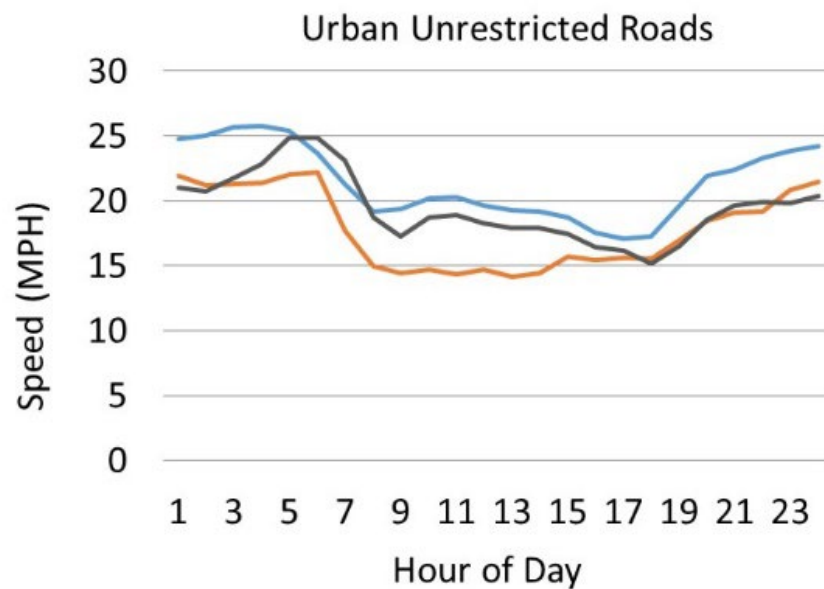
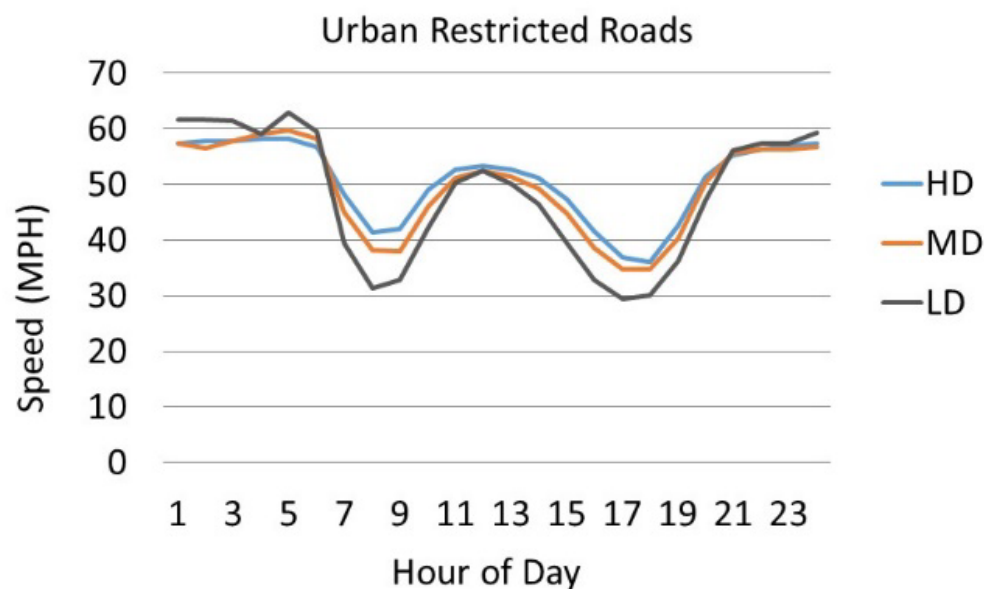
- ▶ Compared Atlanta, Chicago, and Las Vegas
- ▶ Patterns differed by city and from MOVES defaults
 - Weekday patterns for passenger vehicles on urban restricted roads (highways) and unrestricted local roads shown below
 - Note scales differ



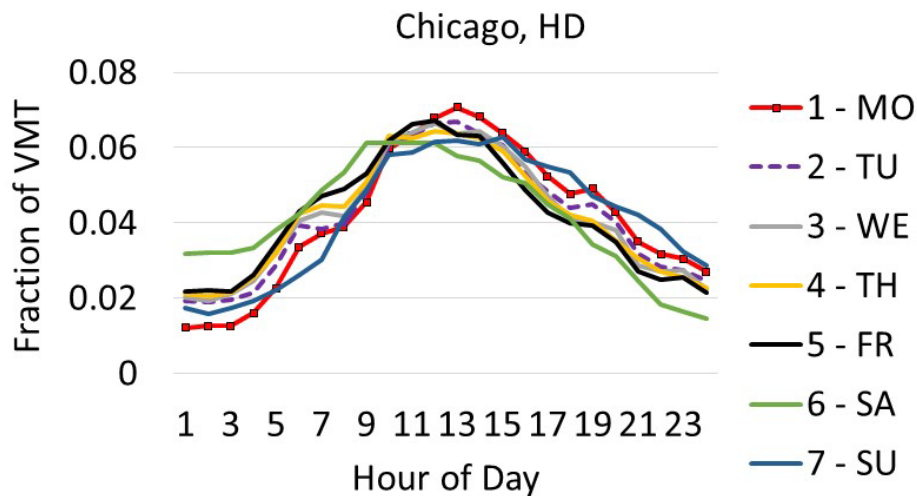
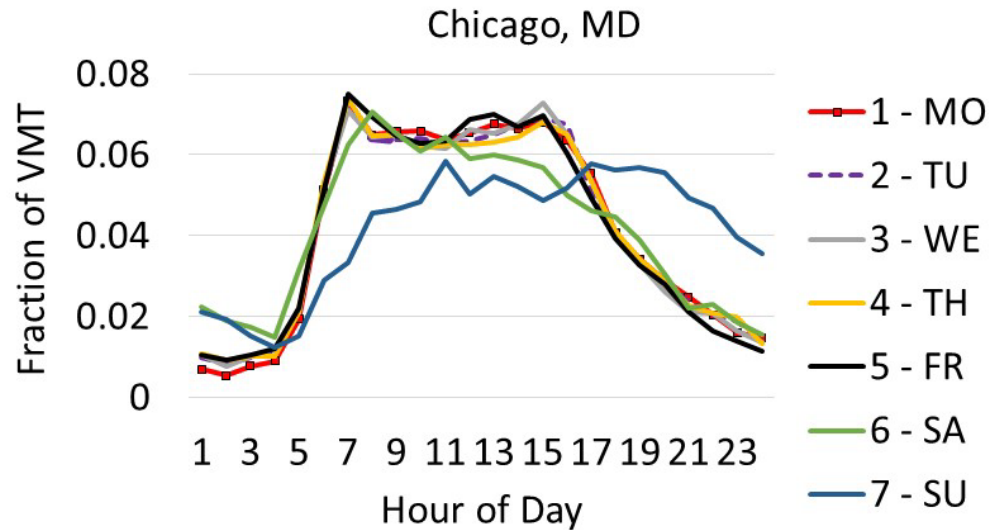
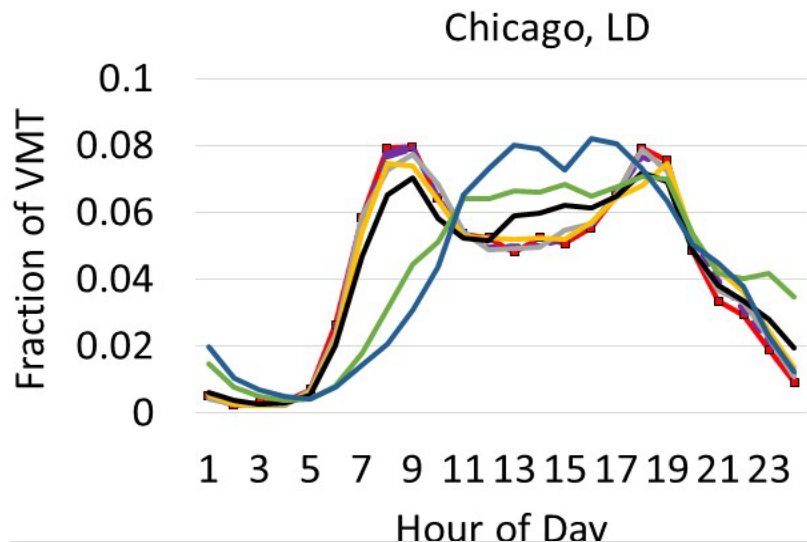


Speed by Vehicle Type

- ▶ Found speed differences between LD, MD, and HD
 - MD/HD speeds higher than LD in many cases
 - Different areas have different patterns esp. on interstates
- ▶ Chicago examples shown below – note scales differ



Diurnal VMT Distributions by Vehicle Type - Chicago example

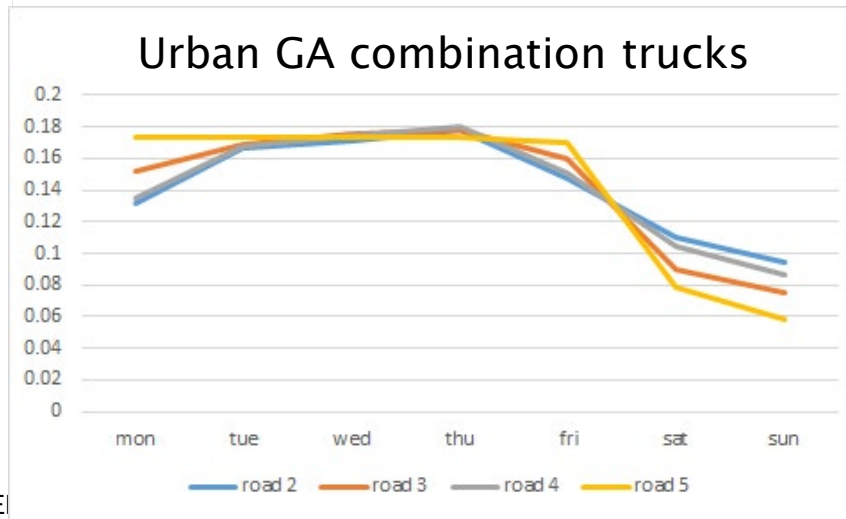
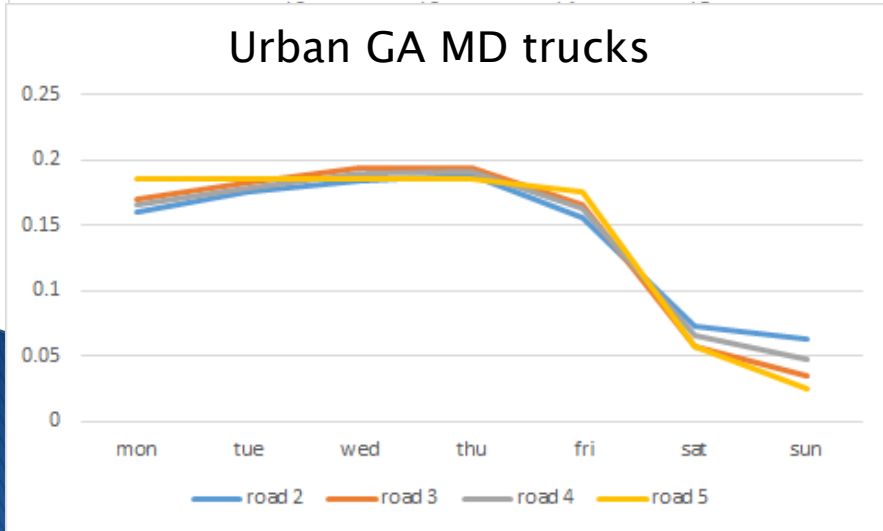
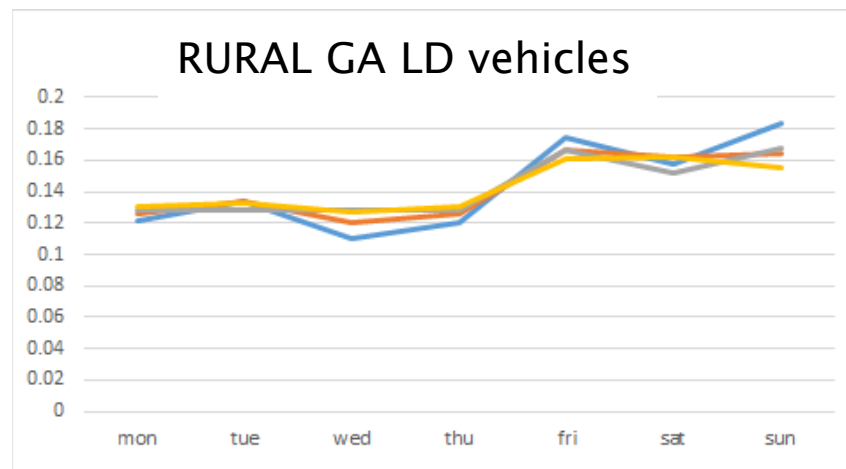
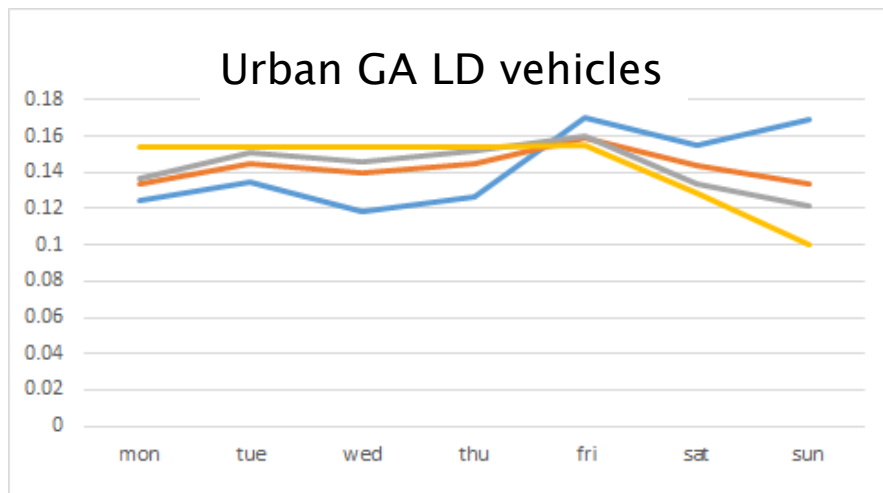


- ▶ Note the differences in patterns weekdays vs weekends and LD/MD/HD
- ▶ Data put into formats to support MOVES (weekday/weekend) and SMOKE (day-specific)



Day of Week Temporal Profiles

- ▶ A-100 data was prepared into MOVES dayVMTFraction and SMOKE day-of-week temporal profiles (SMOKE shown here)



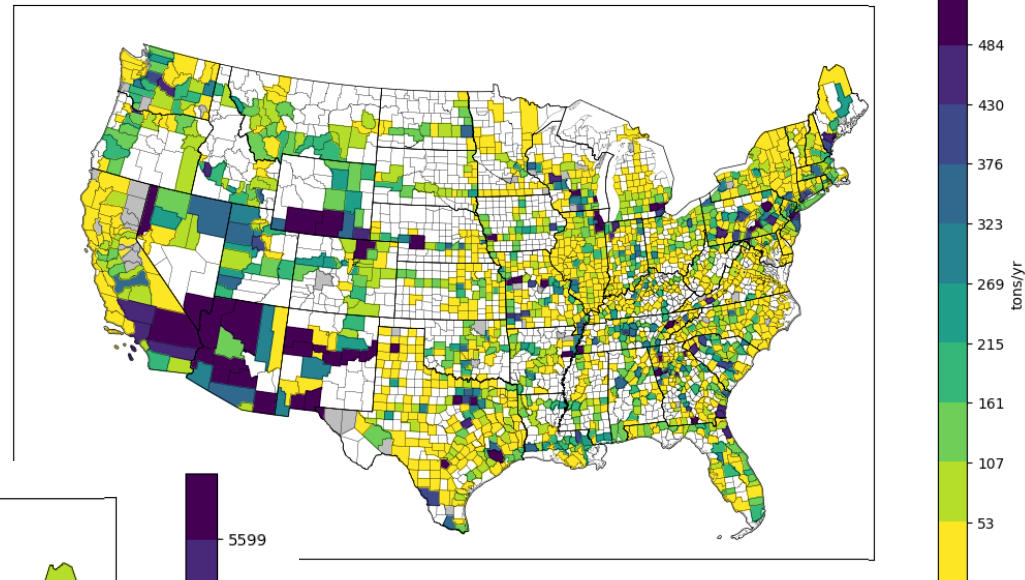
Hoteling and On-roadway NOx by County



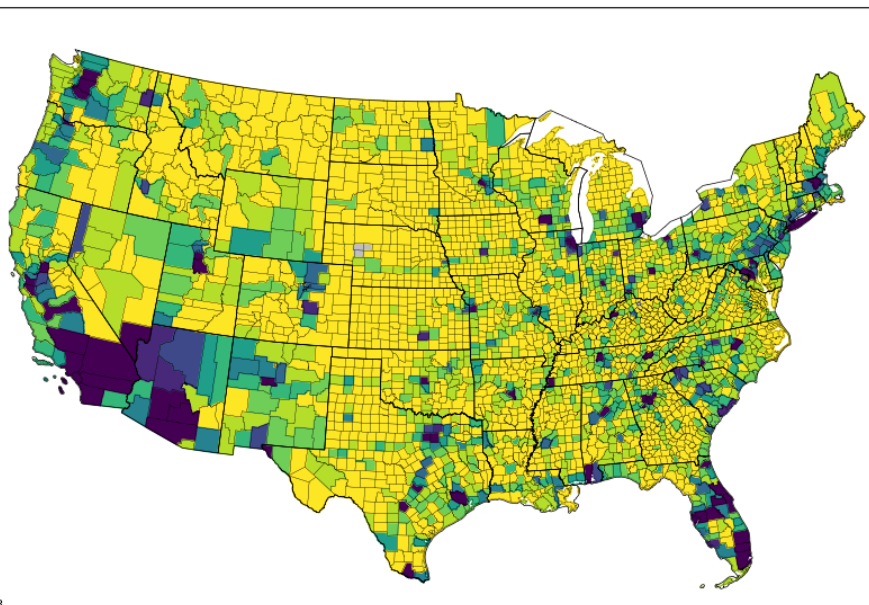
Hoteling follows interstates and has 190K tons NOx (blue=500tpy) ->

Rate per Distance 3.2M tons of 4.1M tons total exists in all counties blue=6000tpy)

2016beta onroad RPH NOX



2016beta onroad RPD NOX



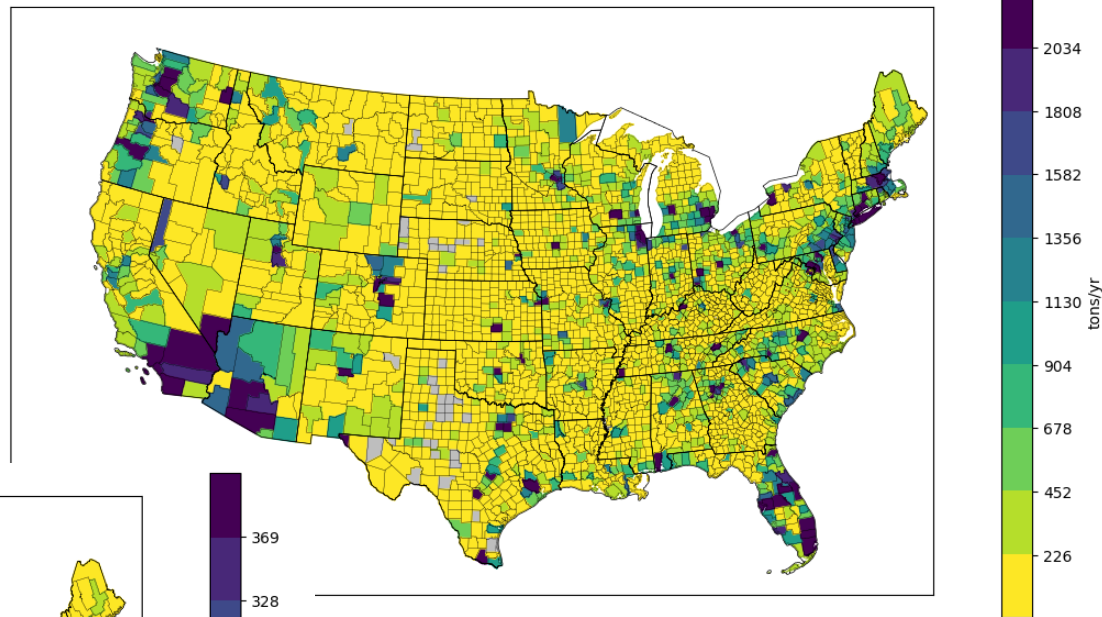
Off-network Emissions by County



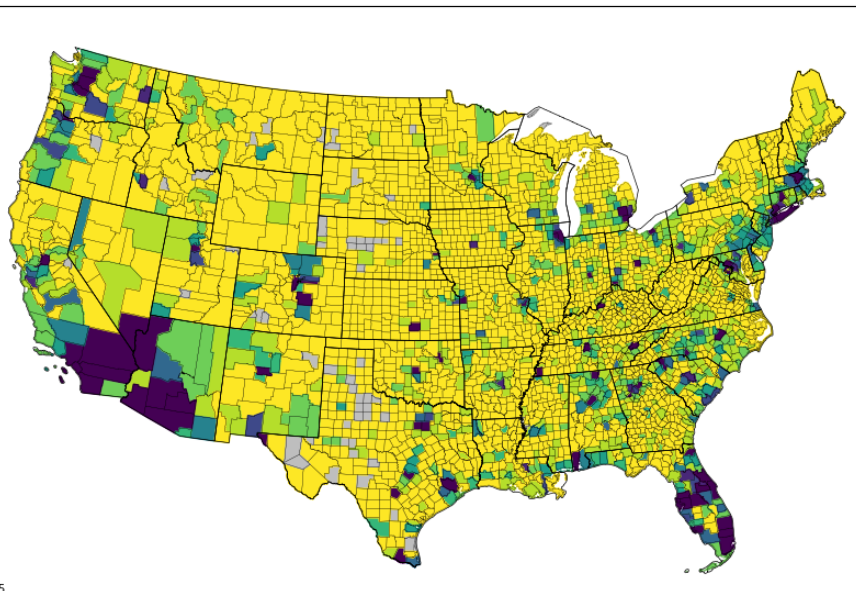
RPV VOC is 1.05M of 2M tons VOC (blue=2000) -> (NO_x=642K of 4.1M tons)

Rate per Profile VOC
180K of 2M tons onroad VOC (blue=370)

2016beta onroad RPV VOC



2016beta onroad RPP VOC

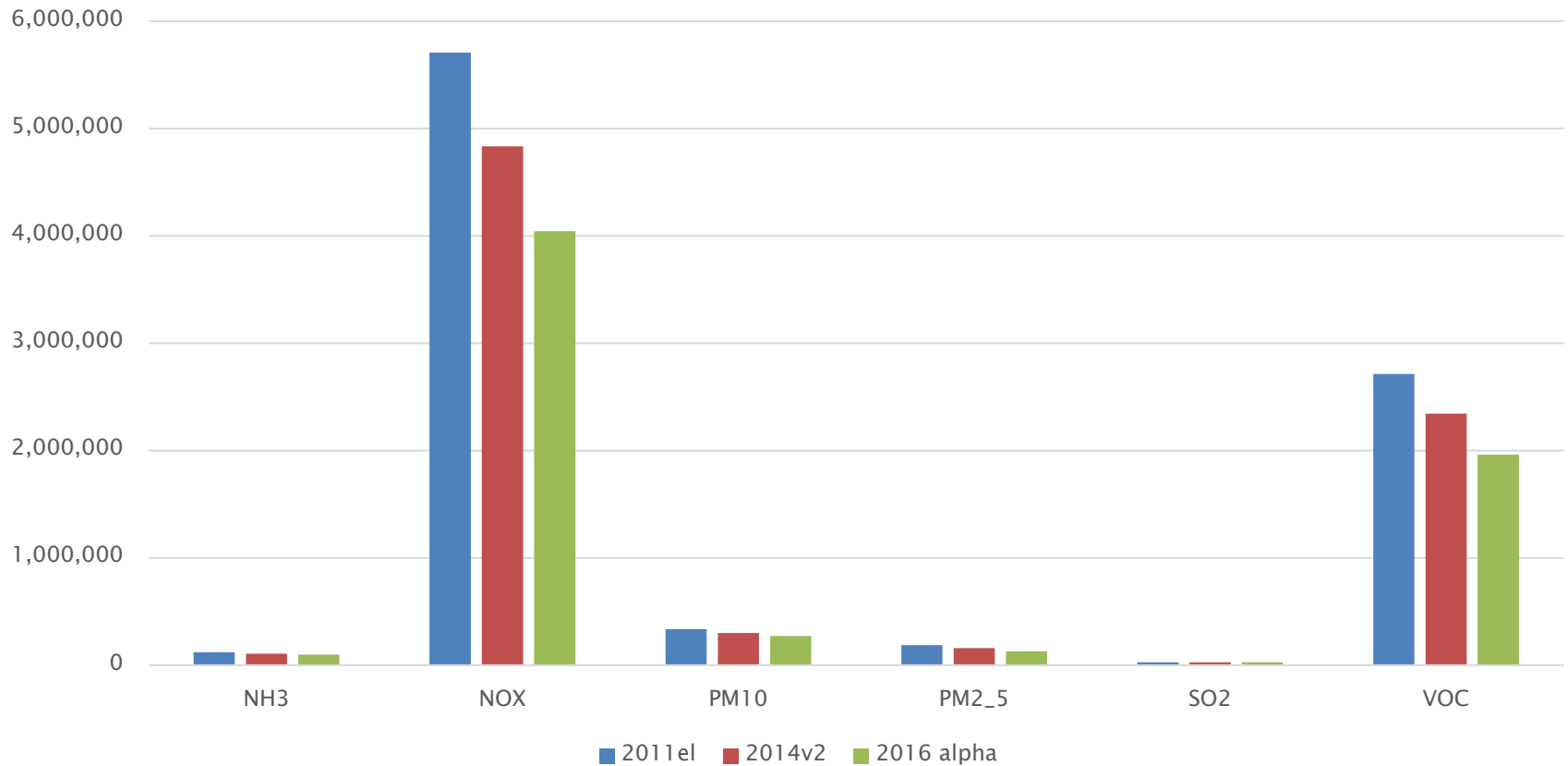


Onroad	NOX	VOC
RPD	3,233,411	720,732
RPH	189,889	35,101
RPP		179,371
RPV	642,240	1,050,560
Total	4,065,540	1,985,763

Onroad Changes 2011 to 2016



Onroad CAP Emissions in 2011, 2014, and 2016



Questions?

- ▶ Any questions on onroad emissions processing?



Commercial Marine Vessels



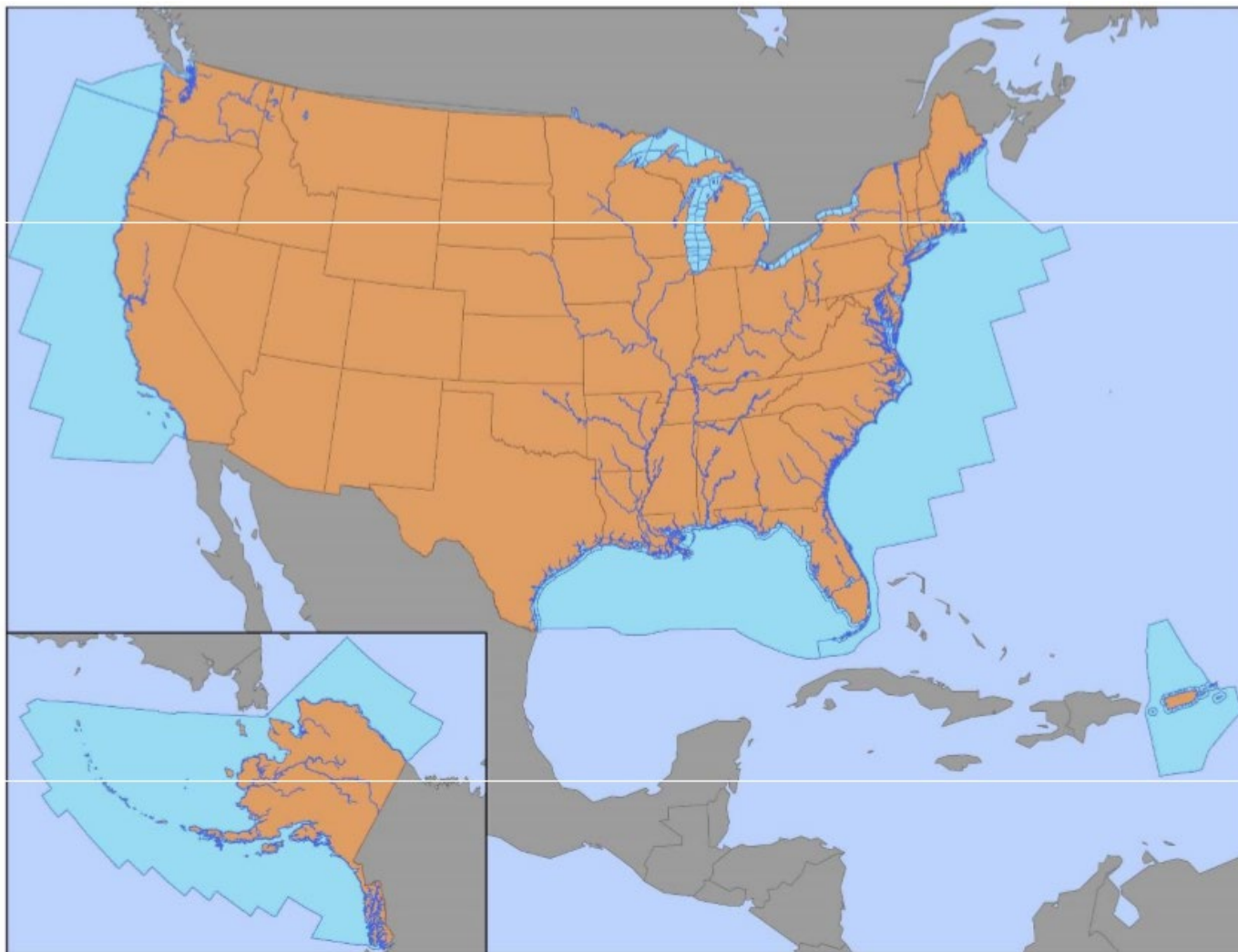
- ▶ CMV in the NEI is split into two broad categories:
 - Category 3 (C3) (i.e., large) vessels with engine displacement above 30 liters that primarily use residual fuel blends
 - C1 and C2 vessels that primarily use distillate fuels
 - Recreational marine vessels are part of nonroad
- ▶ Inventories computed for emissions in state waters (3–10 nautical miles) and federal waters out to 200 nautical miles from the U.S. coastline
 - Port emissions are separated from underway
 - Areas outside of 200 n.m. filled in from non-NEI data sources
- ▶ “Modes” indicate what ships are doing and different emission factors are used for each
 - M=maneuvering, H=hoteling, C=cruise, Z=reduced speed zone
- ▶ EPA data is used except for states that submitted

Commercial Marine Data Sources and Modeling



- ▶ Data sources for CMV in the 2014NEI
 - Entrance and clearance data (2012)
 - About 11,000 vessels linked to routes from origin port to destination port
 - Hours of operation computed based on route and vessel type (e.g., bulk carrier, container, oil tanker) with reduced speed zones factored in
 - Army corps of engineers waterborne commerce data for tugs and barges, bulk carriers, tankers, and other vessels
 - 2007 category 1 and 2 vessel study
 - See 2014NEI TSD for more details
- ▶ Modeling
 - CMV modeling sectors now cmv_c1c2 and cmv_c3 and include all U.S. waters
 - Plume rise computed for cmv_c3 (pseudo-point sources which also help us represent shipping routes)
 - Temporal allocation is mostly flat every hour (except Great Lakes by month)

U.S. State and Federal Waters

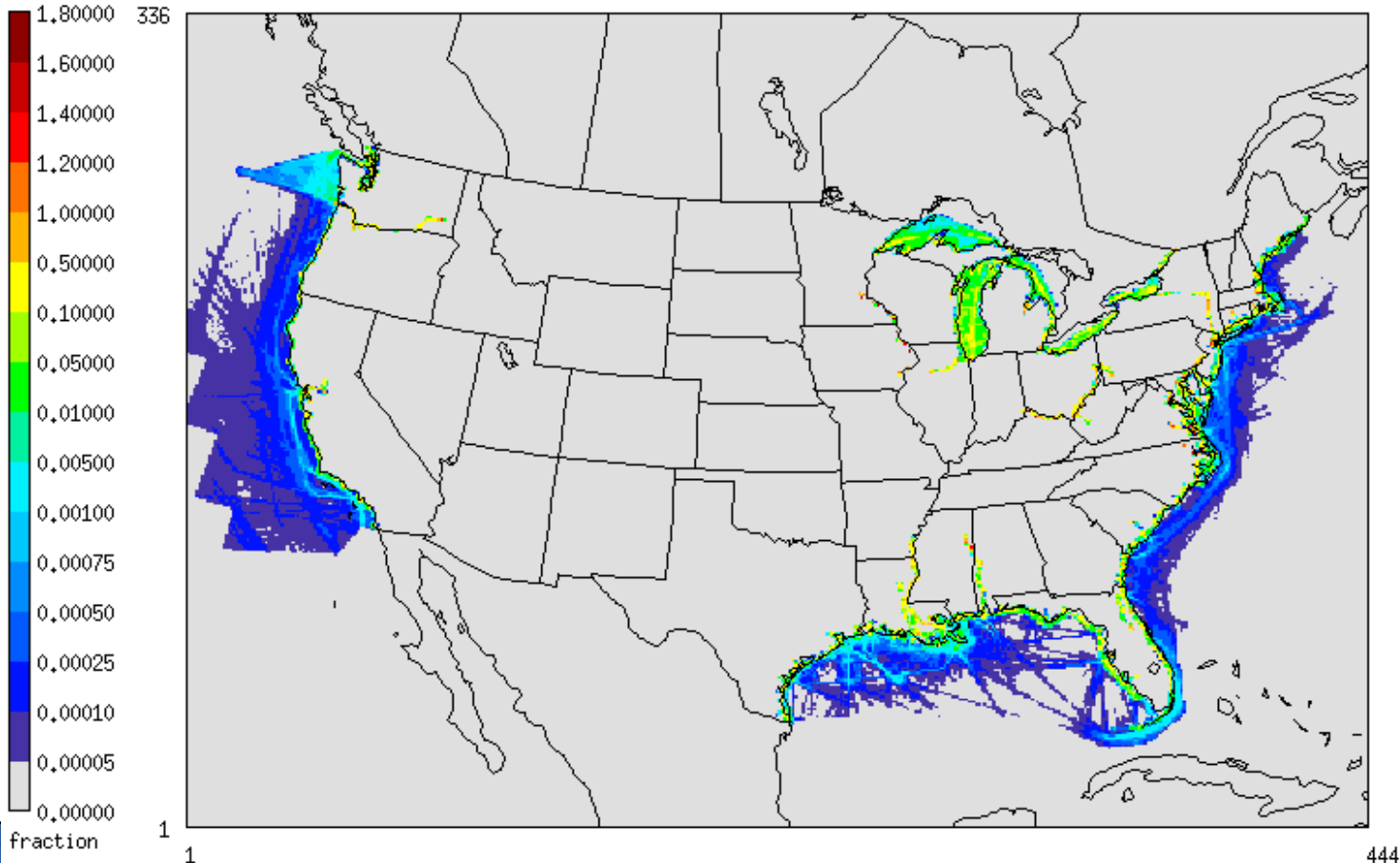


New 12km CMV Spatial Surrogate based on marinecdaster data



FRACTION

NOFILL 12km
USA_808_NOFILL.txt

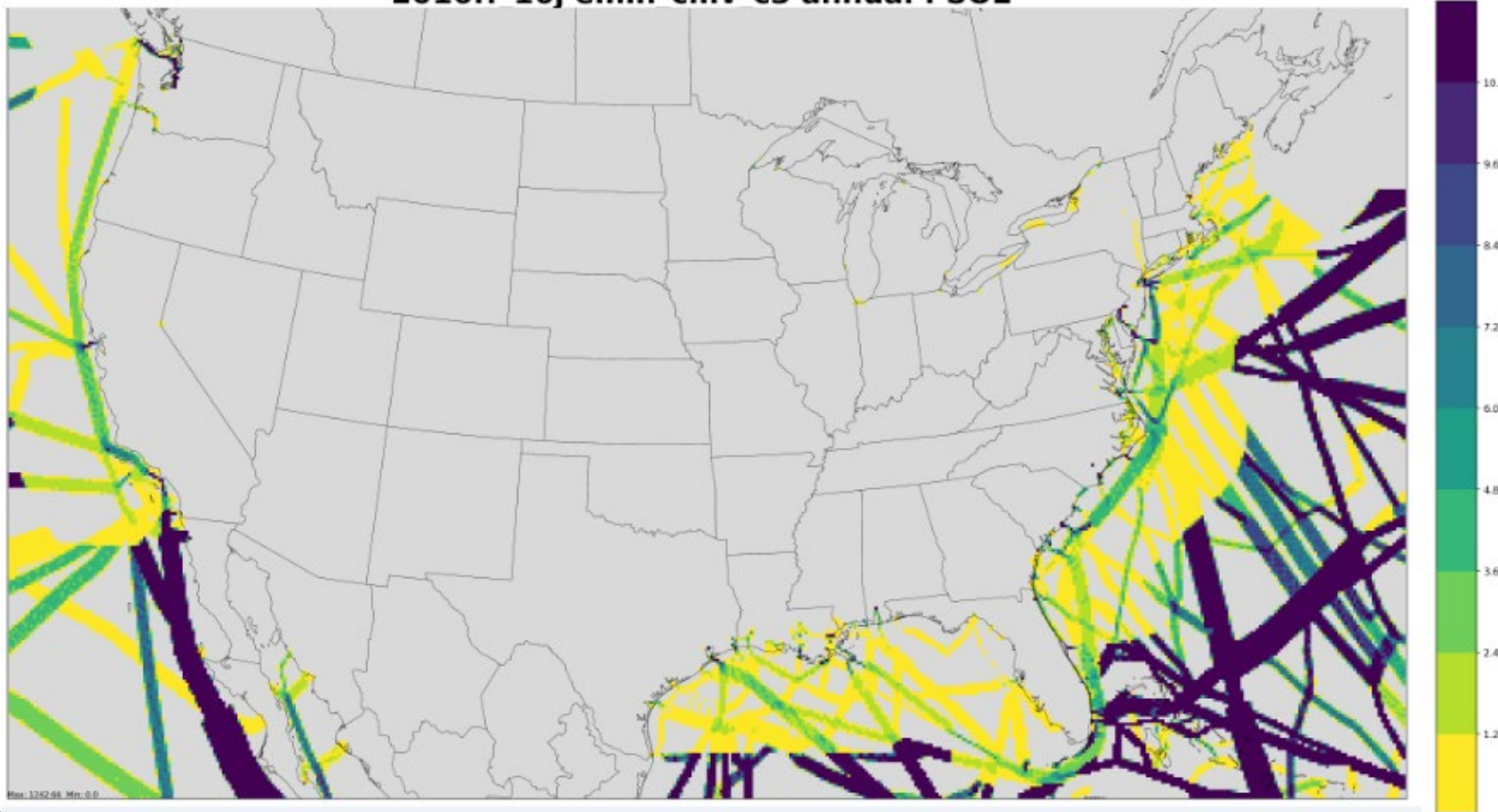


January 1, 2007 0:00:00
Min=0.00000 at (1,1), Max=3.06890 at (387,201)

2016 CMV C3 SO2 Emissions



2016ff 16j emln cmv c3 annual : SO2



Updates to CMV: 2016v1 / 2017 NEI

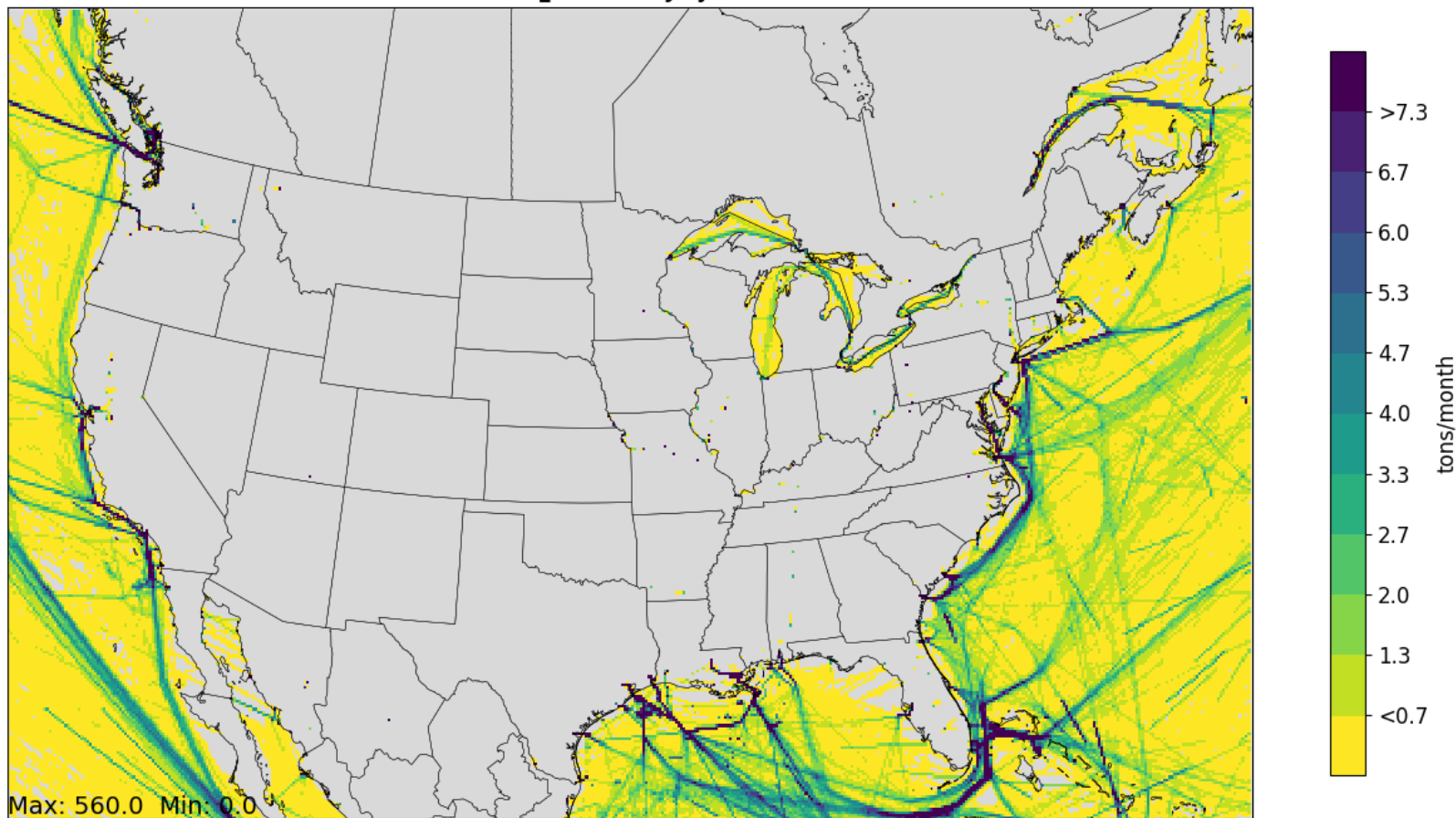


- ▶ CMV for 2016v1 and 2017 NEI are being created based on Automated Identification System (AIS) data
 - Ships have transponders that send signals multiple times per minute
- ▶ AIS data has been obtained for 2017 at 5 minute intervals for U.S. and some Canadian and Mexico Coastal waters
 - Emissions have been computed for 2017 NEI based on ship information and emission factors
 - For modeling, emissions are aggregated by hour and grid cell

July C3 emissions at 12km



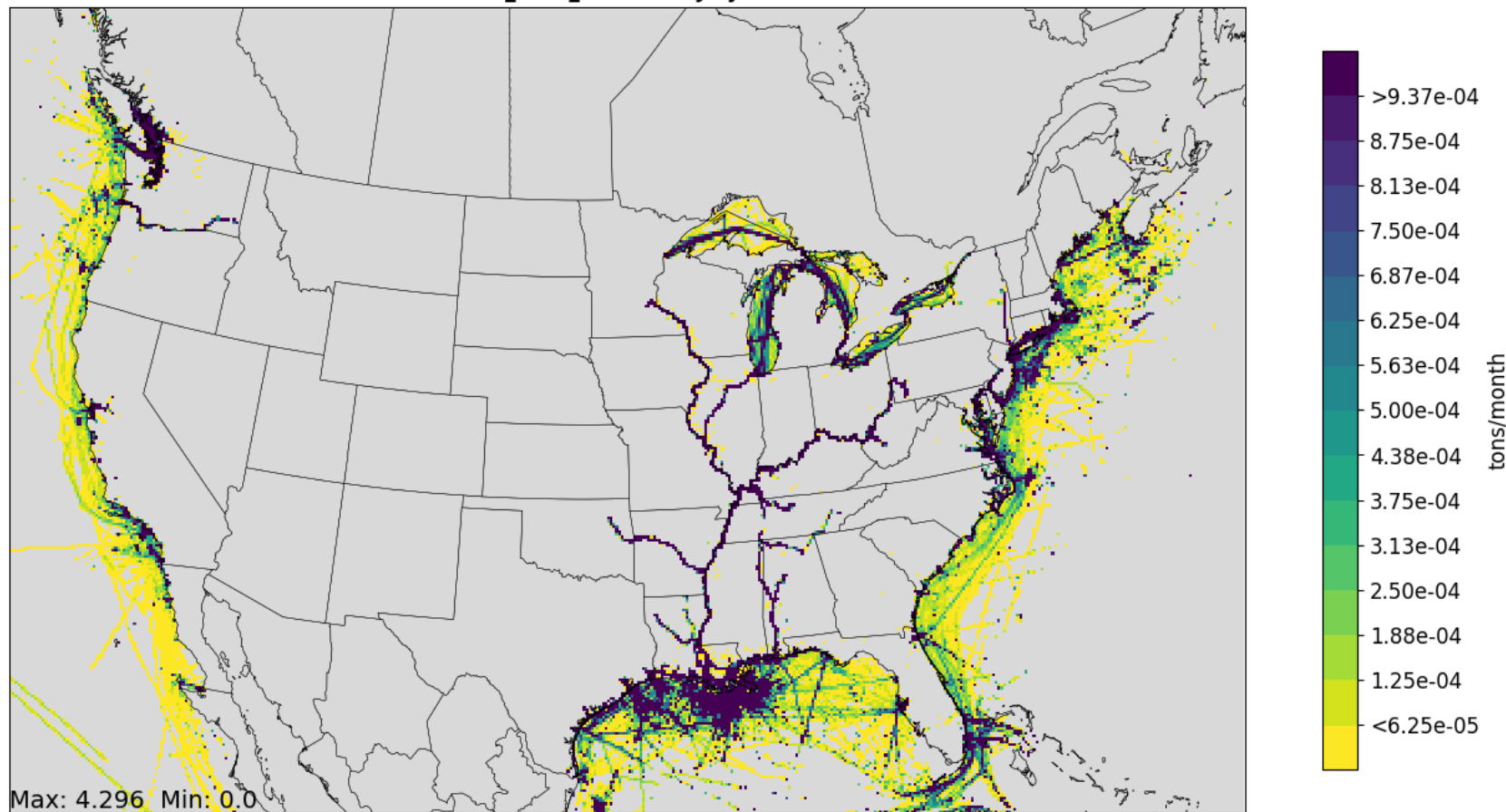
2017 cmv_c3 12US1 July total NOX



July C1C2 Emissions at 12km



2017 cmv_c1c2_12 12US1 July total NOX



Note much lower scale than C3

Questions on CMV?





Modeling 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 – six to eight months
 - Prior year fire emissions used for ramp-up



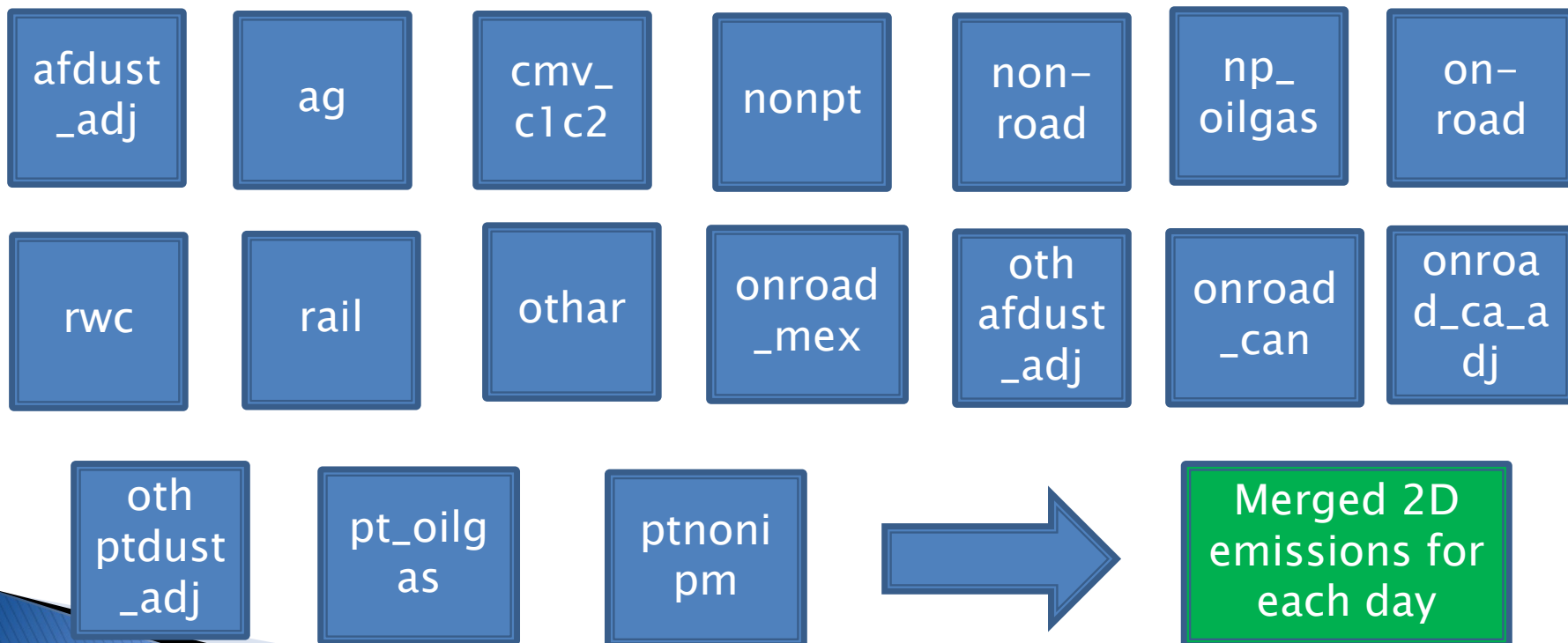
Final Merging and QA

- ▶ After all sectors have been processed through SMOKE programs, the ground-level emissions are merged using the SectorMerge script
 - Runs the mrggrid program based on the Sector list file
 - Only one input for ground-level but point sources can be given to CMAQ by sector without merging
 - cmv_c3, ptegu, ptnonpim, pt_oilgas, ptagfire, ptfire, ptfire_othna, othpt
- ▶ If CAMx is to be run instead of CMAQ, then CAMx conversion scripts must be run
 - CAMx requires point files to be merged



Final Layer 1 Merging

- ▶ All ground-level files must be merged for both CMAQ and CAMx
 - Biogenic emissions can be optionally computed within CMAQ
 - Considers both day-specific and representative day emissions



Ptegu and fire sectors are all elevated

Example Sector List for 2016 Alpha Case



sector	sectorcase	Sectbaseyr	mrgapproach	prevyrspinup	endzip	mergesector
afdust_adj	2016fd_cb6_16j	2016	all	SectBaseYr	Y	Y
ag	2016fd_cb6_16j	2016	all	SectBaseYr	Y	Y
nonroad	2016fd_cb6_16j	2016	mwdss_Y	SectBaseYr	N	Y
rail	2014fd_cb6_16j	2014	aveday_N	SectBaseYr	N	Y
nonpt	2014fd_cb6_16j	2014	week_Y	SectBaseYr	N	Y
np_oilgas	2016fd_cb6_16j	2016	week_Y	SectBaseYr	N	Y
rwc	2016fd_cb6_16j	2016	all	SectBaseYr	Y	Y
ptegu	2016fd_cb6_16j	2016	all	SectBaseYr	Y	Y
ptnonipm	2016fd_cb6_16j	2016	mwdss_Y	SectBaseYr	N	Y
pt_oilgas	2016fd_cb6_16j	2016	mwdss_Y	SectBaseYr	N	Y
ptagfire	2016fd_cb6_16j	2016	all	SectBaseYr	Y	N
ptfire	2016fd_cb6_16j	2016	all	SectBaseYr	Y	N
cmv_c1c2	2014fd_cb6_16j	2014	aveday_N	SectBaseYr	N	Y
ptfire_othna	2016fd_cb6_16j	2016	all	SectBaseYr	Y	N
onroad	2016fd_cb6_16j	2016	all	SectBaseYr	Y	Y
onroad_ca_adj	2016fd_cb6_16j	2016	all	SectBaseYr	Y	Y
othafdust_adj	2016fd_cb6_16j	2016	all	SectBaseYr	N	Y
othar	2016fd_cb6_16j	2016	week_N	SectBaseYr	N	Y
onroad_can	2016fd_cb6_16j	2016	week_N	SectBaseYr	N	Y
onroad_mex	2016fd_cb6_16j	2016	week_N	SectBaseYr	N	Y
othpt	2016fd_cb6_16j	2016	mwdss_N	SectBaseYr	N	N

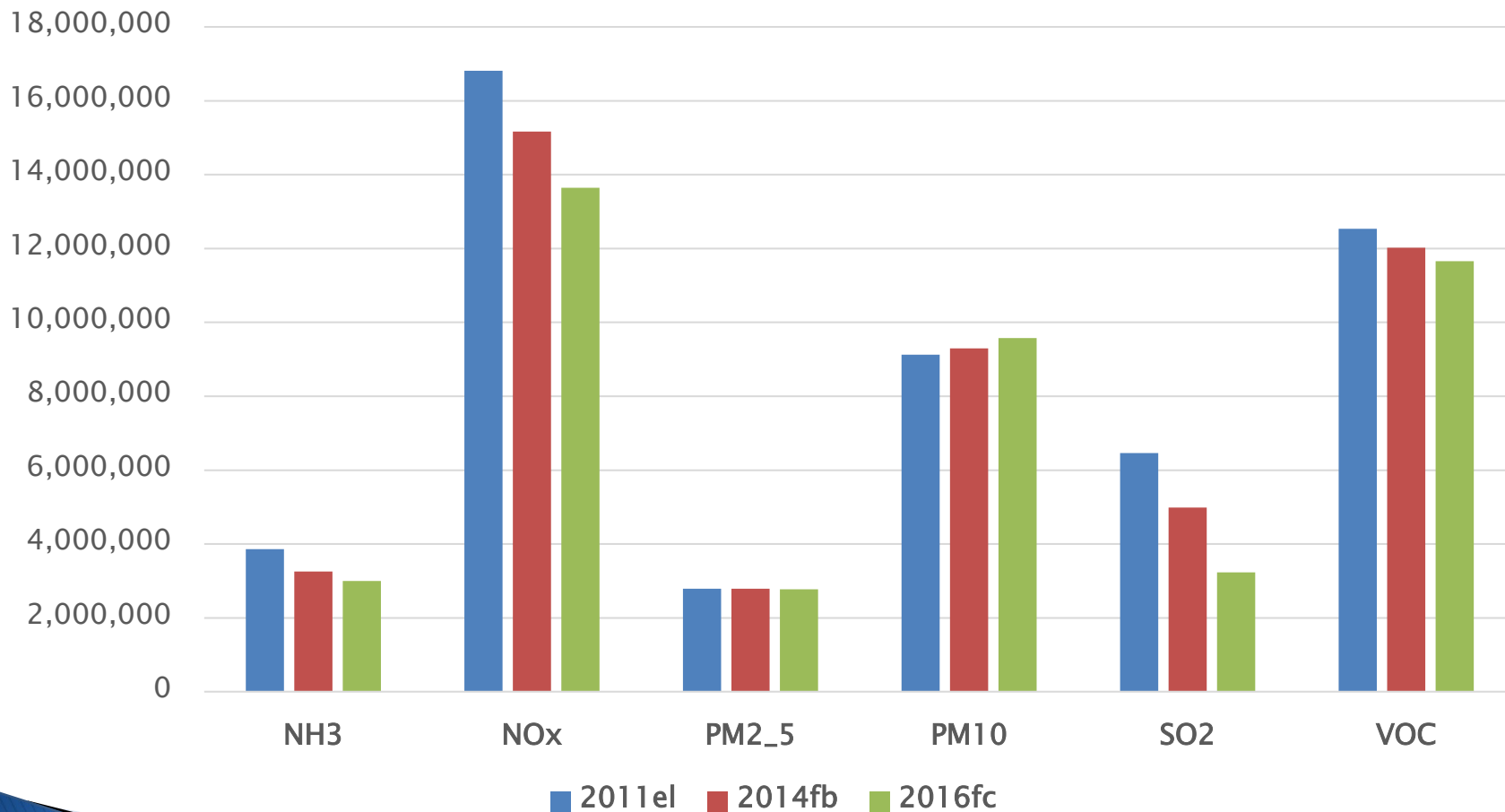
* Some sectors may come from another case



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-specific 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

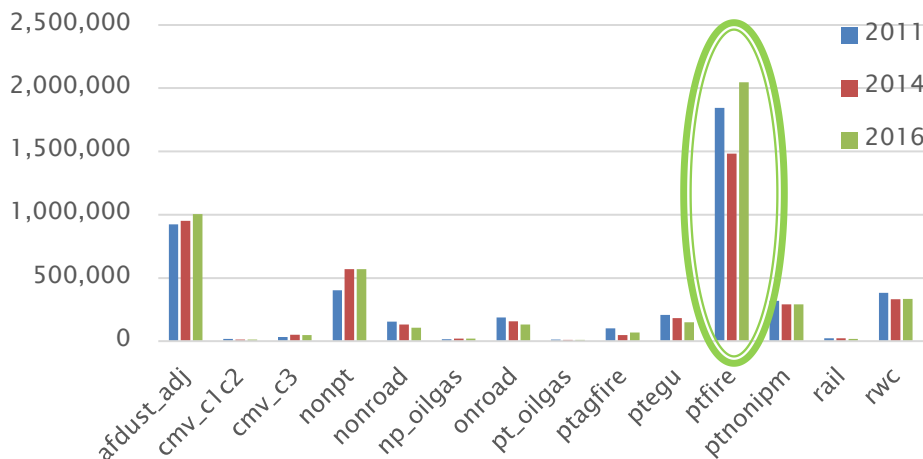
U.S. Base Year Anthropogenic Emissions in 2011, 2014, and 2016



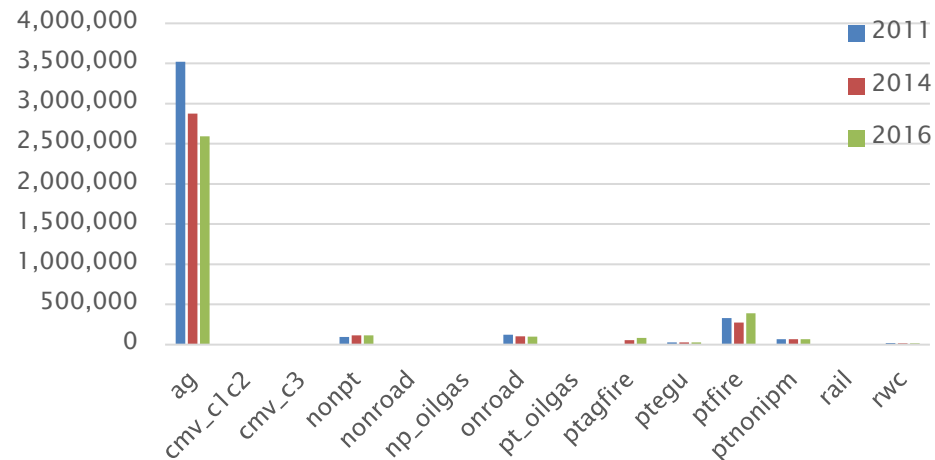
2014 National Emissions by Sector



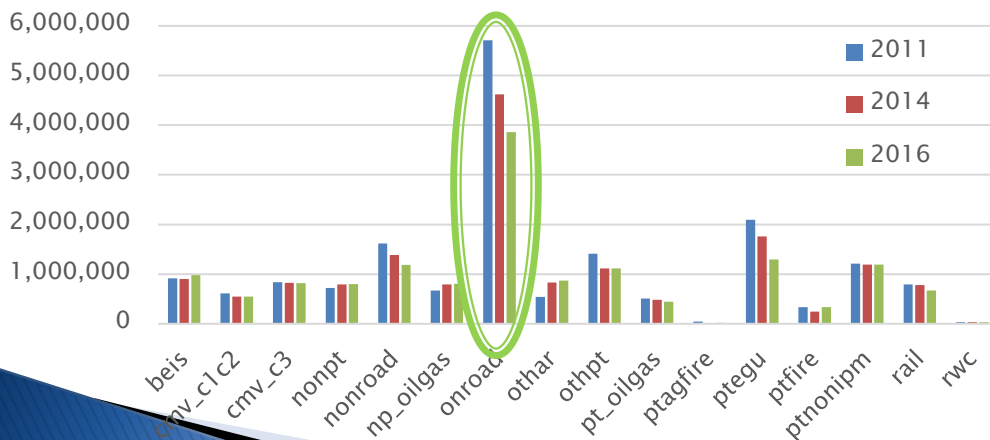
Annual Tons of PM2.5 by Sector



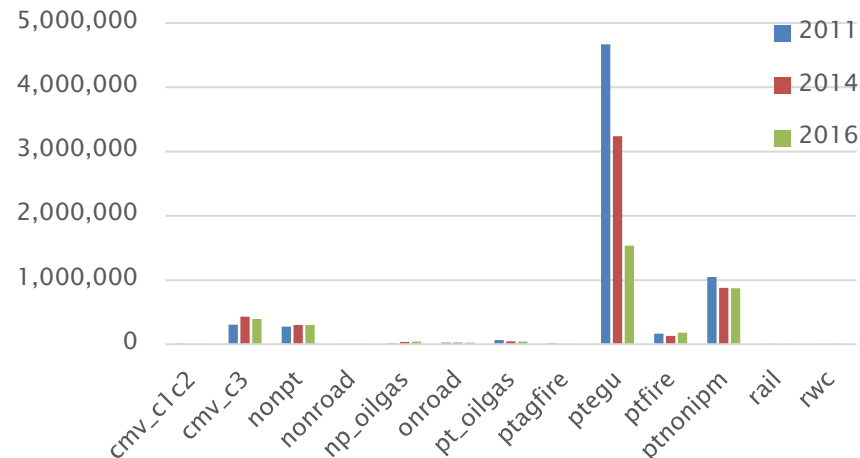
Annual Tons of NH3 by Sector



Annual Tons of NOx by Sector



Annual Tons of SO2 by Sector



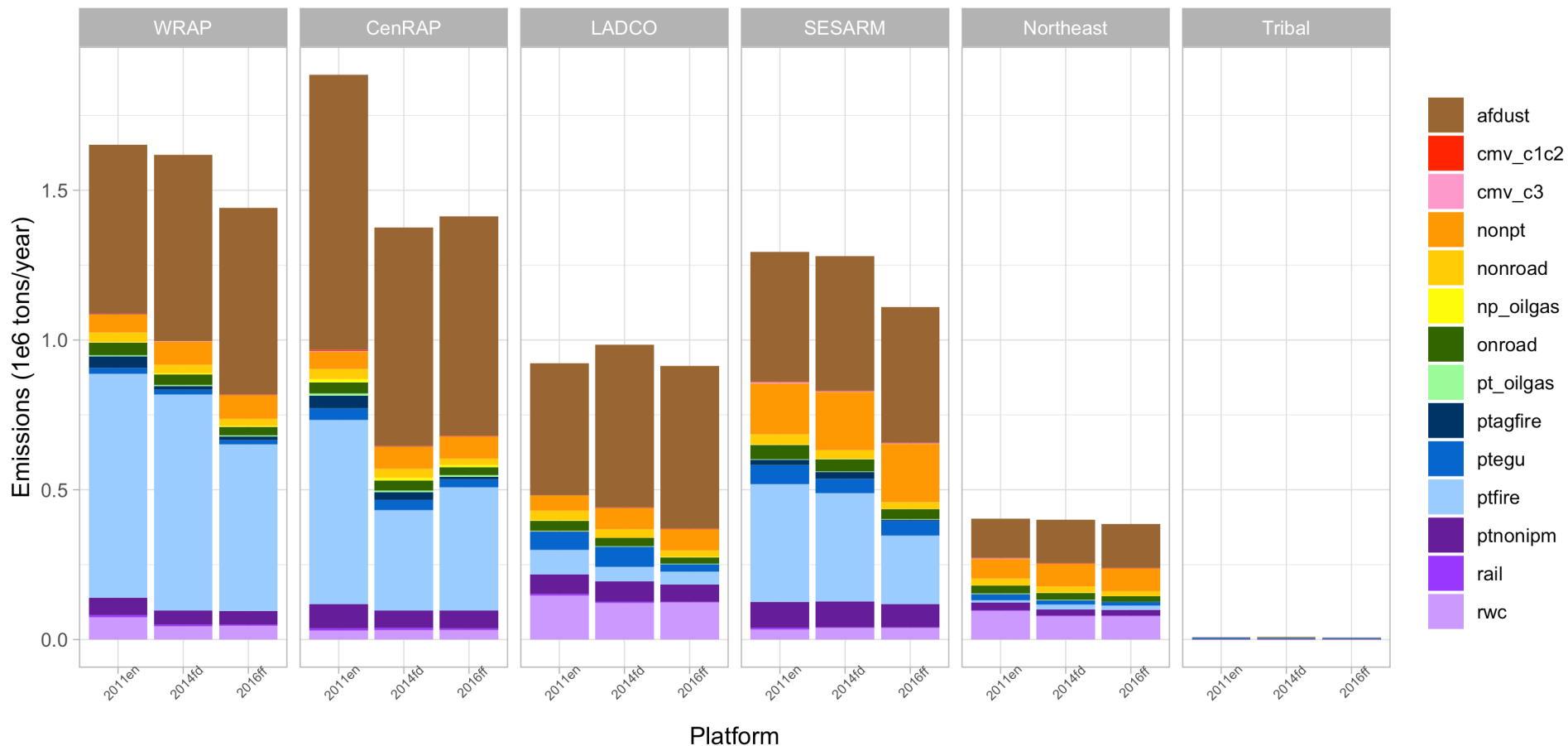
Biogenic emissions comprise 71% of VOCs and fires 8%



2016beta PM2.5 Emissions by Region

Beta Platform Emissions Summary

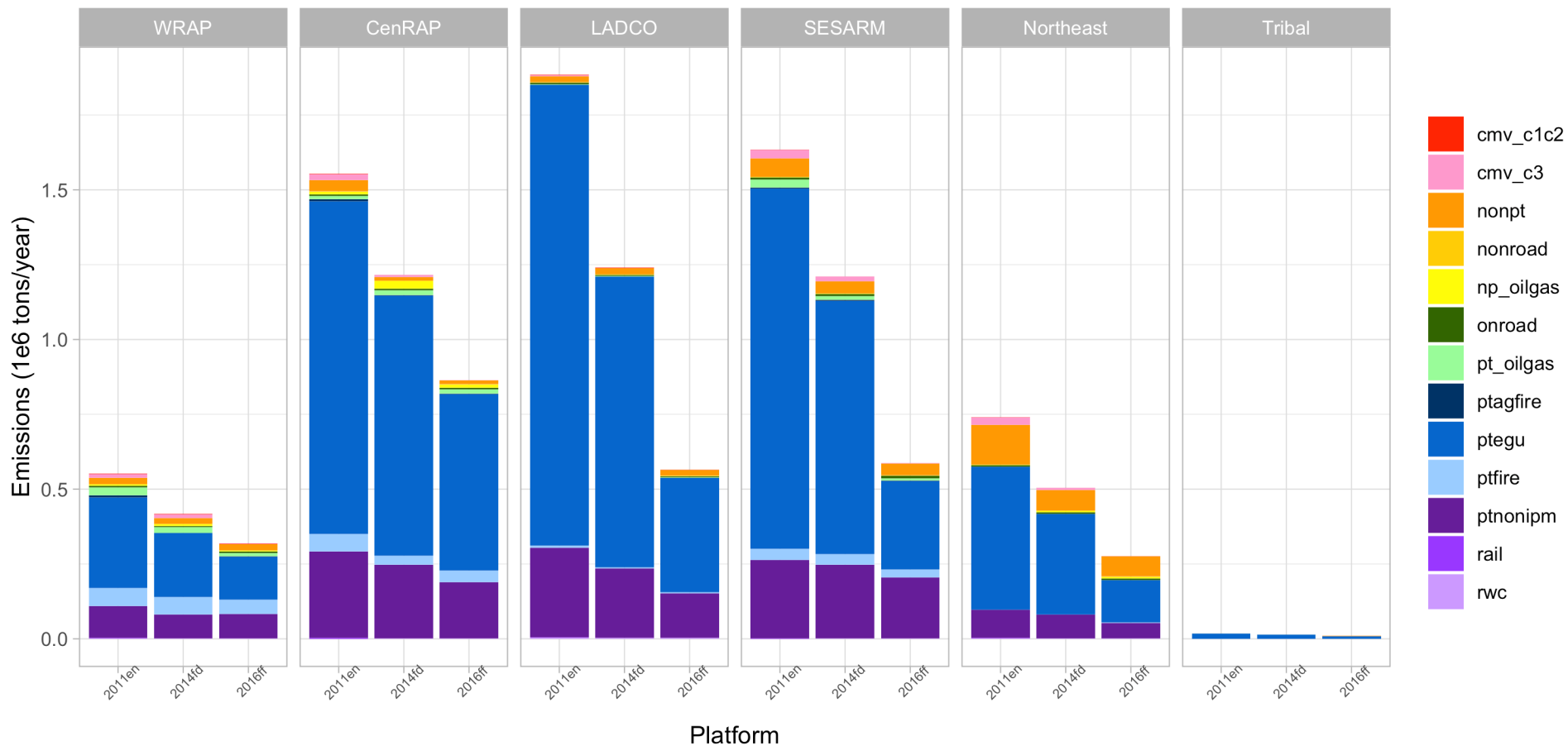
Pollutant: PM25-PRI, Region: US (MJOs/Regions)





2016beta SO2 Emissions by Region

Beta Platform Emissions Summary
 Pollutant: SO2, Region: US (MJOs/Regions)



State-Sector Totals Report



- ▶ State totals by sector before and after SMOKE

2014fa_nata_state_sector_totals.xlsx - Excel

File Home Insert Page Layout Formulas Data Review View ESRI MAPS Tell me what you want to do

Clipboard Font Alignment Number Styles Cells

A3 State

	A	B	C	D	E	F	G	H	I	J	K
1		2014fa Anthropogenic state totals.									
2		CAPs and non-VOC HAPs are inventory-level except onroad (SMOKE-MOVES), afdust (post-adjusted), and ptegu NOX/SO2 (CEM). V									
3	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

Ready



CAMx Conversion

- ▶ EPA always prepares the emissions files initially using CMAQ's netCDF format
- ▶ Scripts are provided to convert to CAMx:
 - Map species from CMAQ model ready names to CAMx names
 - Convert Merged gridded 2D emissions are from netCDF (IOAPI) format to CAMx model ready format "emis2d" files
 - Merge gridded CAMx emissions with met-based surf zone sea-salt emissions files
 - Convert inline CMAQ model ready emissions to CAMx point "ptsr" emissions for each sector
 - This step requires that fires have been processed in 3D
 - Merge the CAMx point "ptsr" emissions into a single point "mrgpt" file for the CAMx model



Source apportionment

- ▶ Source apportionment (SA) is used for transport and sector-based 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 source apportionment runs
- ▶ A standalone 2-D sea-salt file is read by CAMx (all others are in CAMx ptsr format)

Emissions Modeling Platform Data Availability



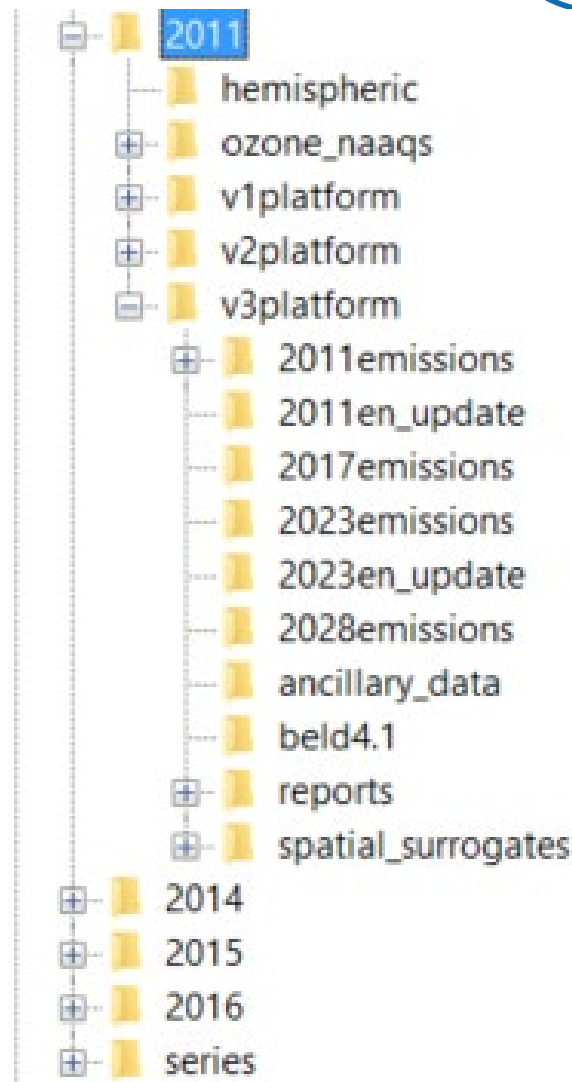
- ▶ EPA's modeling platform data, documentation, scripts available from
 - <https://www.epa.gov/air-emissions-modeling>
 - Version 6 platforms include:
 - 2011v6.3: January 2017 NODA (2011el/2023el), Final Cross-State Air Pollution Rule (CSAPR) Update (2011ek/2017ek), hemispheric case
 - Version 7.0 platform for NATA based on 2014NElv1
 - 2016 alpha platform with compatible 2014 and 2015
 - Spatial surrogates available for 4km, 12km, 36km
 - Speciation data for CB05, CB6, SAPRC07TB
 - Temporal profiles for all sectors

Emissions Modeling FTP site



Several versions of the 2011 platform plus versions of 2014, 2015, and 2016 are available on the FTP site:

<ftp://newftp.epa.gov/air/emismod>



2016 Beta Emissions and Summary Reports on EPA FTP site



Index of /Air/emismod/2016/beta/

[parent directory]

Name	Size	Date Modified
2016emissions/		4/30/19, 9:37:00 AM
ancillary_data/		5/10/19, 7:27:00 AM
draft_emissions/		3/5/19, 9:46:00 AM
met_for_emissions/		5/6/19, 9:08:00 AM
reports/		4/9/19, 9:22:00 AM
spatial_surrogates/		2/28/19, 10:49:00 AM

Index of /Air/emismod/2016/beta/2016emissions/

[parent directory]

Name	Size	Date Modified
point_split_by_state/		4/8/19, 5:21:00 AM
2016_beta_platform_2016ff_updates_043019.tar.contents.txt	3.0 kB	4/29/19, 1:07:00 PM
2016_beta_platform_2016ff_updates_043019.tar.gz	930 MB	4/29/19, 1:08:00 PM
2016ff_inventory_allocation_update_30apr2019.zip	557 MB	4/30/19, 9:36:00 AM
2016ff_inventory_allocation_update_30apr2019_contents.txt	3.0 kB	4/30/19, 9:36:00 AM
2016ff_inventory_cem_17dec2018.zip	235 MB	3/19/19, 8:56:00 AM
2016ff_inventory_cem_17dec2018_contents.txt	2.9 kB	3/19/19, 8:56:00 AM
2016ff_inventory_fires_02jan2019.zip	437 MB	3/19/19, 8:56:00 AM
2016ff_inventory_fires_02jan2019_contents.txt	7.4 kB	3/19/19, 8:56:00 AM
2016ff_inventory_nonpoint_01feb2019.zip	512 MB	3/19/19, 8:56:00 AM
2016ff_inventory_nonpoint_01feb2019_contents.txt	3.8 kB	3/19/19, 8:56:00 AM
2016ff_inventory_nonroad_06dec2018.zip	1.7 GB	3/19/19, 8:58:00 AM
2016ff_inventory_nonroad_06dec2018_contents.txt	443 B	3/19/19, 8:58:00 AM
2016ff_inventory_onroad_activity_02jan2019.zip	35.6 MB	3/19/19, 8:58:00 AM
2016ff_inventory_onroad_activity_02jan2019_contents.txt	1.1 kB	3/19/19, 8:58:00 AM
2016ff_inventory_oth_02jan2019.zip	1.8 GB	3/19/19, 8:59:00 AM
2016ff_inventory_oth_02jan2019_contents.txt	3.7 kB	3/19/19, 8:59:00 AM
2016ff_inventory_point_02jan2019.zip	145 MB	3/19/19, 8:59:00 AM
2016ff_inventory_point_02jan2019_contents.txt	1.4 kB	3/19/19, 8:59:00 AM

Additional information is available on the 2016 beta Wiki page:

<http://views.cira.colostate.edu/wiki/wiki/10197>

Final Questions before lunch?



- ▶ Any final questions on the base year part of the training?



- ▶ Contacts: eyth.alison@epa.gov,
farkas.caroline@epa.gov,
Vukovich.jeffrey@epa.gov