Preparing Emissions for Air Quality Modeling

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Course Outline

- 8:00 Background, Inventories, Tools, and QA
- 8:30 Spatial Allocation
- 8:45 Temporal Allocation
- 9:00 Speciation
- 9:20 Processing for biogenics, EGUs, and Onroad
- 9:45 Break
- 10:00 Projections Overview
- 10:15 EGU Projections
- 10:30 Nonroad and Onroad Mobile Projections
- 11:00 Non-EGU Projections
- 11:35 Limitations, New Directions, and Questions
- 11:45 End of Class

Goal of Class

- To introduce you to the various tasks involved with preparing emissions inputs to air quality models
- To answer commonly asked questions about this process

Background: Purpose and Contents of a Modeling Platform

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

Common Air Quality Studies

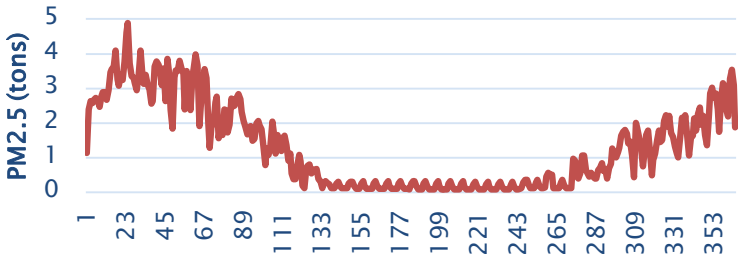
- Regulatory Impact Assessments
  - Model a base year (includes CAPs plus a few HAPs)
  - Model a future year base case with on-the-books rules
  - Model one or more cases that represent the rule
  - Estimate costs and benefits of rule
- National Air Toxics Assessment
  - Focus on HAPs
  - Model a base year with as many HAPs as possible
  - Compute risk
- Transport Modeling
  - Model a base year and future year base case
  - Perform source apportionment modeling to determine contribution of states to nonattainment in other states

Emissions Modeling Process

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

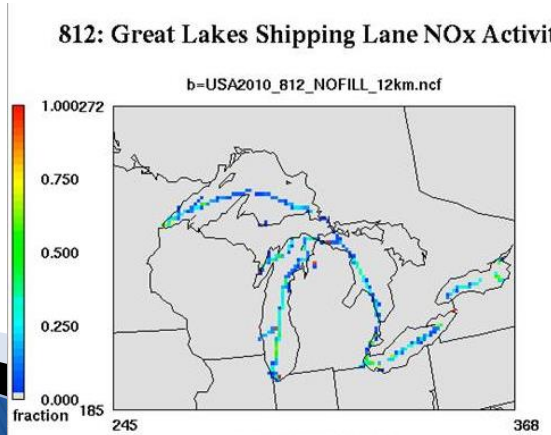
Inventories (annual/ monthly/daily)

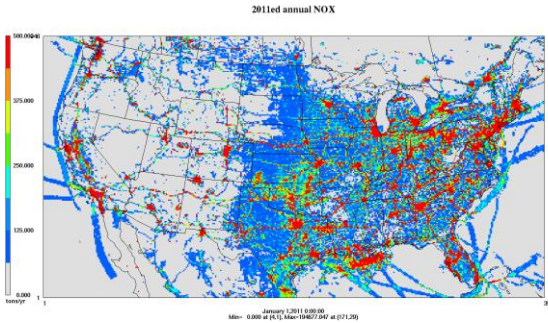
Temporal Profiles



Speciation Profiles

Spatial Surrogates



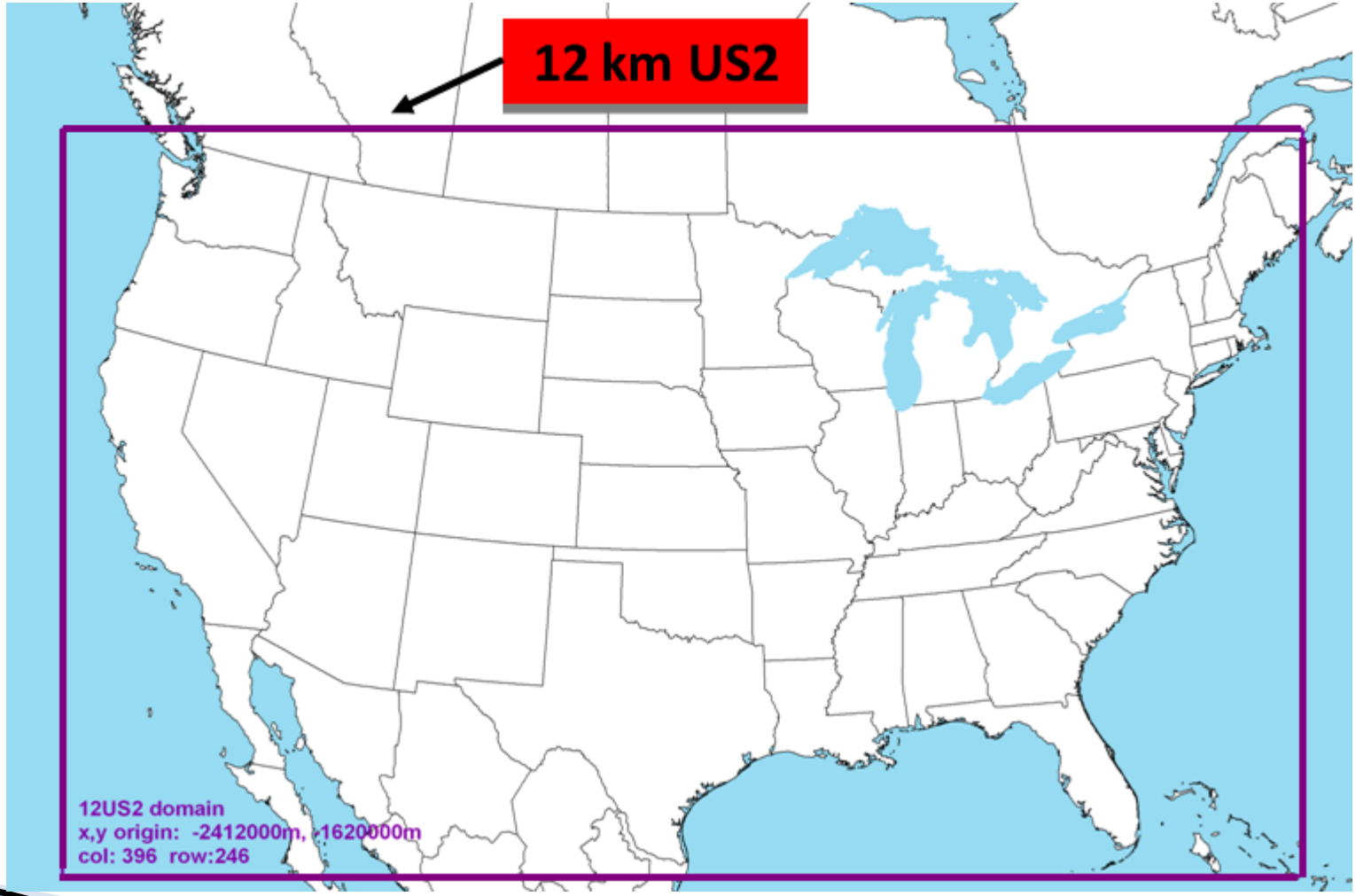


Gridded, hourly, speciated emissions for air quality modeling

Performing Emissions Modeling

- We use the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system (http://cmascenter/smoke) and associated tools to process our emissions into air quality model-ready files
- The starting emission inventories (e.g., NEI) can be annual, monthly, daily, or hourly
- Other "ancillary" data files help process inventories into files containing hourly emissions in model grid cells, and using the chemical species (e.g., NO, NO_2, ISOP) that match the air quality model
- Meteorological data is needed to compute the emissions for some sectors using information on temperature, precipitation, and radiation (e.g., onroad mobile, biogenics)
- Quality assurance steps and data summaries are important
  - Make sure data is properly transformed and that no mass is unexpectedly lost during processing

2011 Platform Modeling Domain



Base Year Emissions: 2011 National Emissions Inventory

- Data is submitted by states, locals, tribes (S/L/T) and EPA into the Emissions Inventory System
- Five categories
  - Point/Facility Inventory (point locations)
  - Nonpoint (county-based)
  - Onroad mobile sources
  - Nonroad mobile sources
  - Events (e.g., Fires)
- EPA and S/L/T data are blended to create the NEI
  - http://www.epa.gov/ttn/chief/net/2011inventory.html
- **2011 NEI Version 2 released in March!**

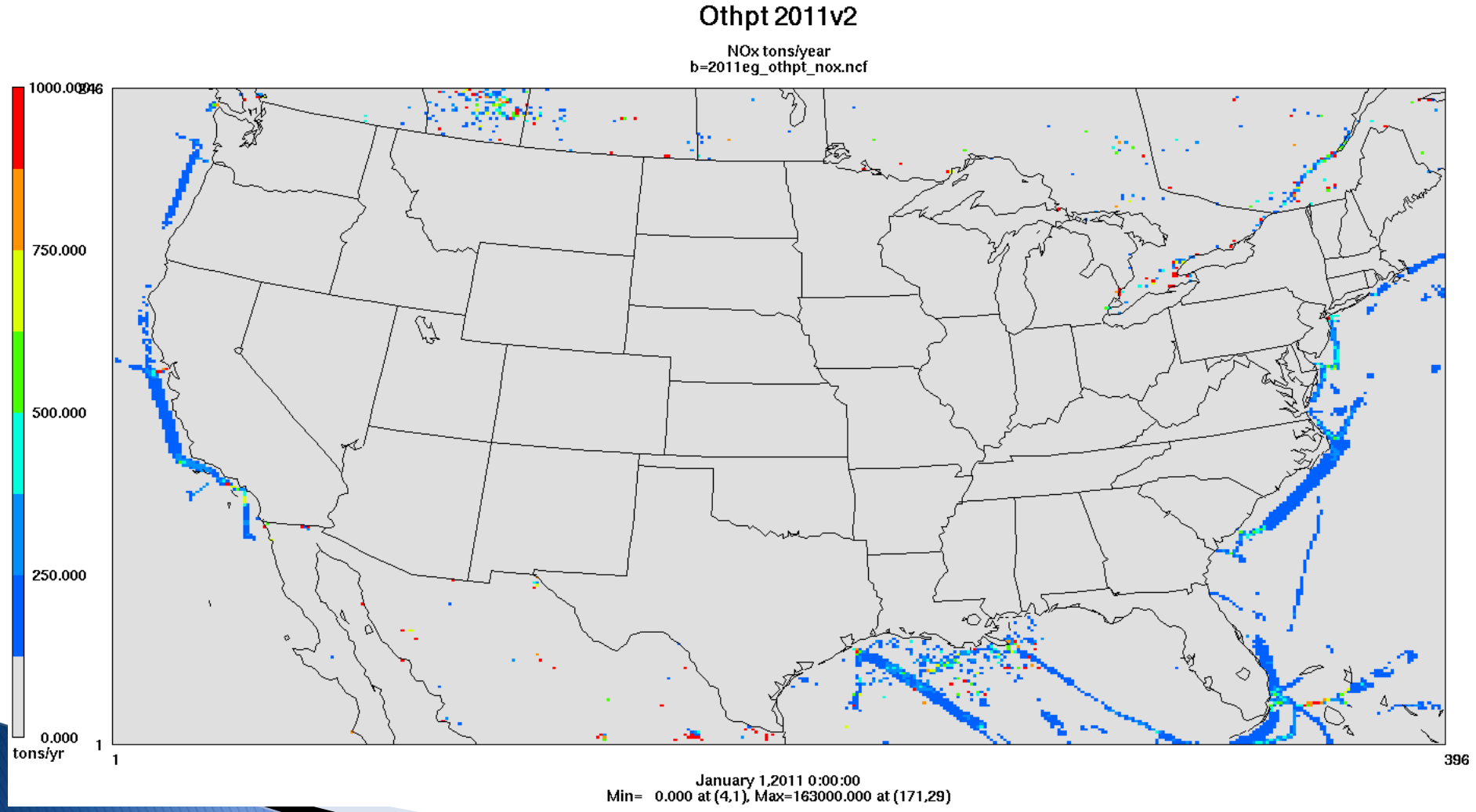
Recent Emission Inventory Updates to 2011 Modeling Platform

- U.S. emissions based on 2011 NEI Version 2
  - Includes revisions submitted by states / locals / tribes
  - Further revisions obtained through NATA review process
  - MOVES 2014 for onroad emissions plus new SCCs
  - Oil and gas tool / inventory updates from EPA and states
  - Residential wood combustion updates
  - Agricultural burning reductions in the Midwest
  - Redistribution of Commercial Marine Vessel emissions
  - Gulf of Mexico emissions updated to 2011
  - Updated biogenic emissions based on BEIS v3.6.1
- Numbering system for platform differs from NEI
  - Newest platform is 2011v6.2 (2008NEI platforms=v5.x)
  - New cases use later letters (2011ed, 2011eg, 2011eh)

Non-US emissions included in the platform

- Canada 2010 emissions & spatial surrogates (courtesy Environment Canada)
- Mexico 2008 emissions – compiled from the Inventario Nacional de Emisiones de Mexico, 2008
- Biogenic emissions in Canada and Mexico are computed as part of the standard processing
- 2011 fire emissions in Canada and Mexico provided by Western Regional Air Partnership (WRAP), but not yet used in our modeling

2011v2 Platform NOx Point Sources Outside of State Boundaries



Emissions Modeling Platform Sectors and Data sources

- **EPA processes emissions separately for each sector then merges them:**
- ag: nonpoint agricultural emissions (primarily ammonia)
- afdust: area fugitive dust (NEI NP – only PM)
- c1c2rail: Category 1 and 2 commercial marine + railroads (NEI NP)
- c3marine: Category 3 commercial marine vessels in state waters (NEI NP)
- rwc: residential wood combustion (NEI NP)
- nonpt: nonpoint emissions not in other sectors (NEI NP)
- beis: biogenic emissions (model in SMOKE: Normbeis3, Tmpbeis3)
- onroad: onroad mobile sources (on and off-network from SMOKE-MOVES)
- nonroad: nonroad mobile sources (NEI nonroad, but monthly)
- ptegu: EGU point sources (NEI point)
- pt_oilgas: point oil and gas (NEI point)
- ptnonipm: non-EGU point sources (NEI point – not EGUs or oil and gas)
- ptfire: includes wild and prescribed fires as point sources (NEI events)
- othpt: point emissions outside of state waters (Can, Mex, oil platforms, CMV)
- othar: non-US nonpoint and nonroad emissions (Can, Mex, marine traffic)
- othon: non-US onroad emissions (Can, Mex)

Platform Data not in the NEI

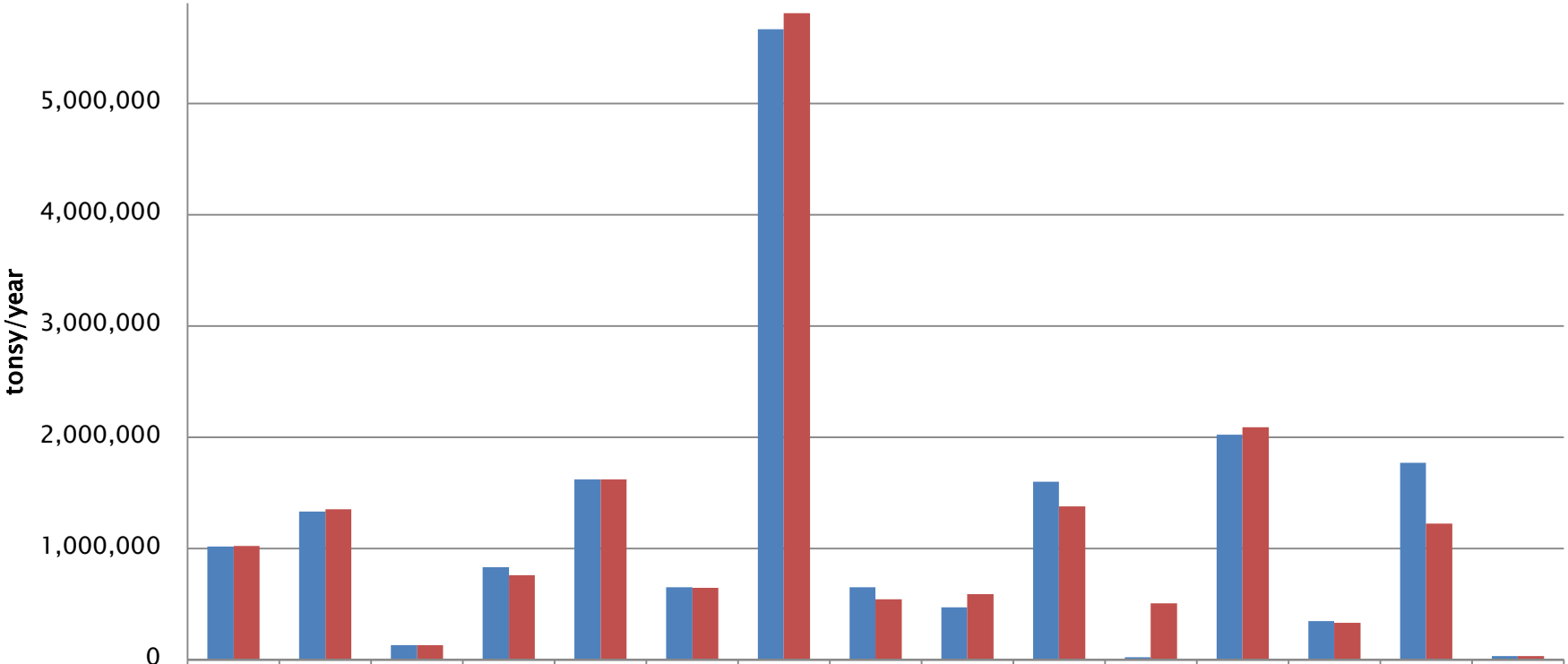
- Sometimes the platform uses data not in the NEI
  - Correct issues are found after the NEI release
  - New data becomes available after NEI release
  - More detailed data is available than NEI stores
    - Continuous Emissions Monitoring System (CEMS) data for EGUs
    - Nonroad data is monthly (summed for NEI)
    - Onroad and biogenics data is hourly (summed for NEI)
  - NEI uses average meteorological adjustments, but platform uses hourly, gridded met. data (e.g., afdust sector)

Building a Platform

- When a new NEI version becomes available, we get a flat file from EIS and split the point and nonpoint inventories into sectors
  - Onroad, nonroad, and biogenics done before NEI release
- Typically, when we build a new platform, we compare the inventories and results based on any new methods to a previous platform
  - Difference reports by state, county, and if needed SCC
  - Charts and maps
- Examples of other assessments done as needed
  - Sub-annual (e.g. ozone season, hourly, daily)
  - Examine speciated PM or VOC
  - Review gridded inventory emissions

Note the sectors that contribute most, and largest differences

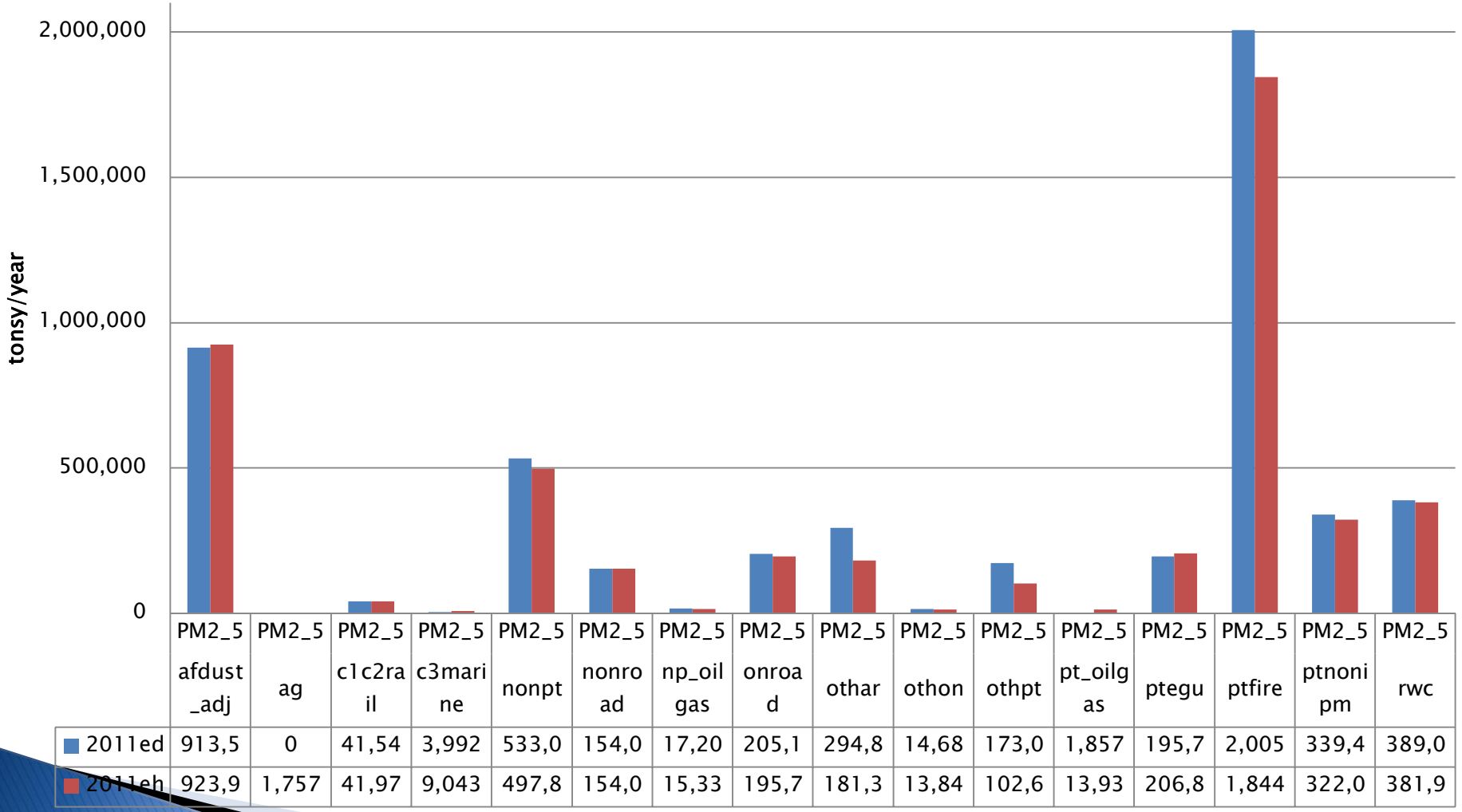
NOX in 2011eh (v2) vs 2011ed (v1)



	NOX beis	NOX c1c2rail	NOX c3marine	NOX nonpt	NOX nonroad	NOX np_oilgas	NOX onroad	NOX othar	NOX othon	NOX othpt	NOX pt_oilgas	NOX ptegu	NOX ptfire	NOX ptnonipm	NOX rwc
2011ed	1,017,	1,331,	131,30	831,25	1,620,	653,21	5,666,	652,58	469,08	1,597,	22,091	2,023,	347,10	1,771,	35,758
2011eh	1,020,	1,354,	131,38	762,29	1,620,	647,14	5,809,	544,76	589,37	1,376,	509,84	2,088,	333,40	1,222,	34,508

North Carolina reduced fire emissions > 90%

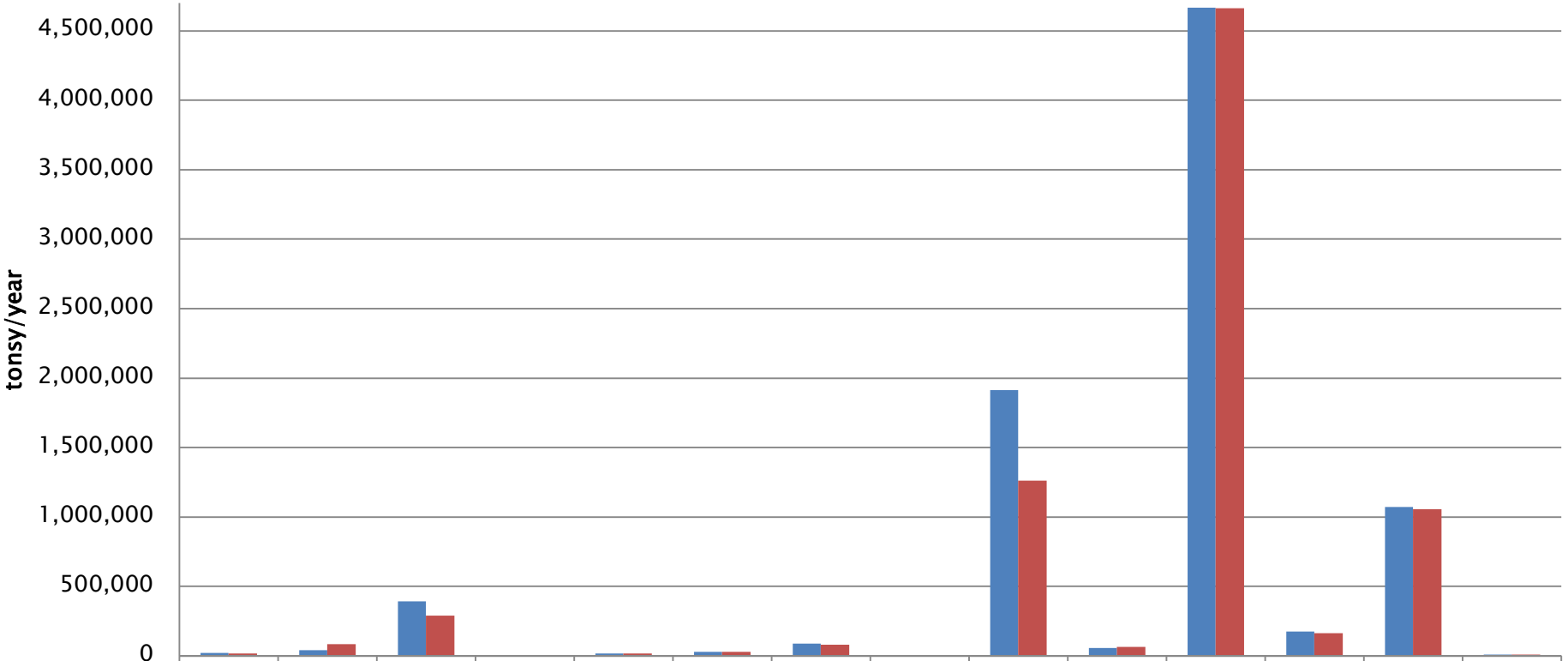
PM2_5 in 2011eh (v2) vs. 2011ed (v1)



	PM2_5 afdust_adj	PM2_5 ag	PM2_5 c1c2rail	PM2_5 c3marine	PM2_5 nonpt	PM2_5 nonroad	PM2_5 np_oilgas	PM2_5 onroad	PM2_5 othar	PM2_5 othon	PM2_5 othpt	PM2_5 pt_oilgas	PM2_5 ptegu	PM2_5 ptfire	PM2_5 ptnonipm	PM2_5 rwc
2011ed	913,5	0	41,54	3,992	533,0	154,0	17,20	205,1	294,8	14,68	173,0	1,857	195,7	2,005	339,4	389,0
2011eh	923,9	1,757	41,97	9,043	497,8	154,0	15,33	195,7	181,3	13,84	102,6	13,93	206,8	1,844	322,0	381,9

Non-US SO2 went down a lot; nonpt also down some

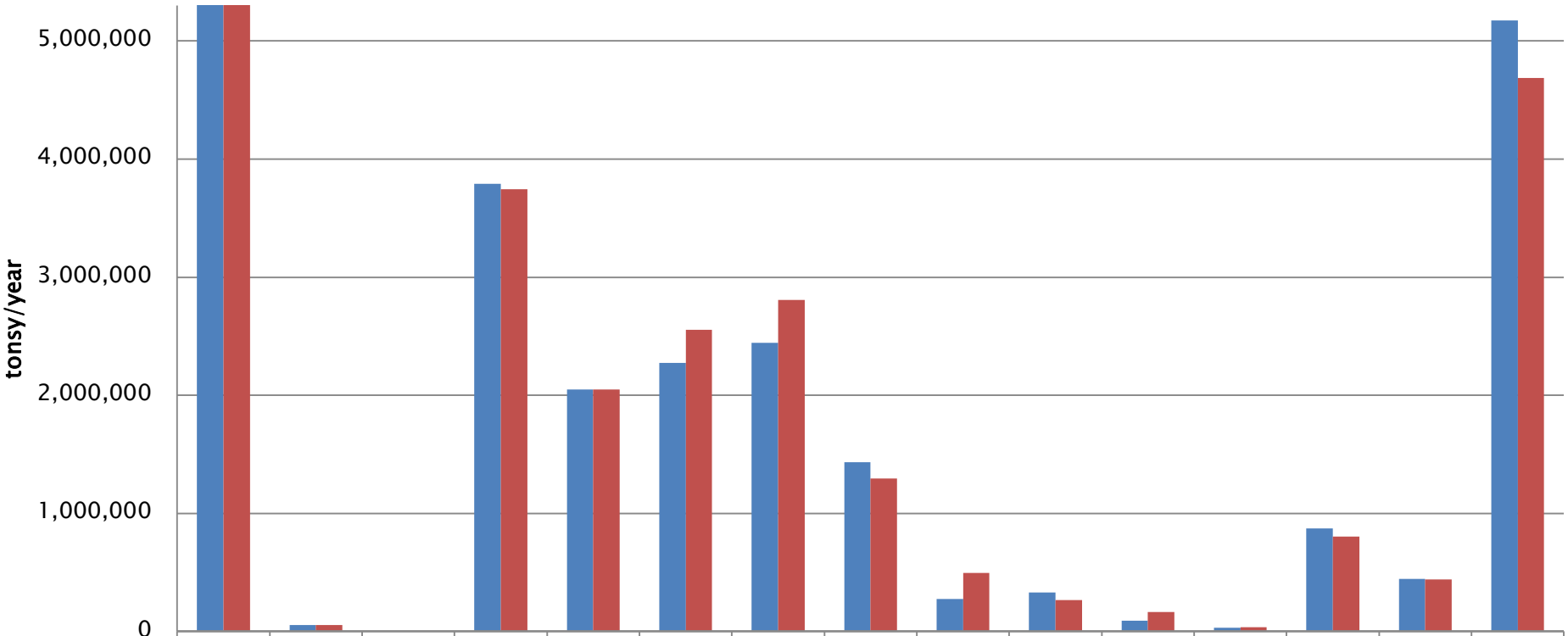
SO2 in 2011eh (v2) vs. 2011ed (v1)



	SO2 c1c2rail	SO2 c3marine	SO2 nonpt	SO2 nonroad	SO2 np_oilgas	SO2 onroad	SO2 othar	SO2 othon	SO2 othpt	SO2 pt_oilgas	SO2 ptegu	SO2 ptfire	SO2 ptnonipm	SO2 rwc
2011ed	22,418	40,692	392,00	4,011	17,195	27,915	87,738	5,459	1,915,	55,273	4,665,	177,12	1,071,	9,000
2011eh	16,039	86,373	291,46	4,011	18,310	29,109	80,951	6,621	1,261,	66,576	4,662,	165,79	1,057,	8,964

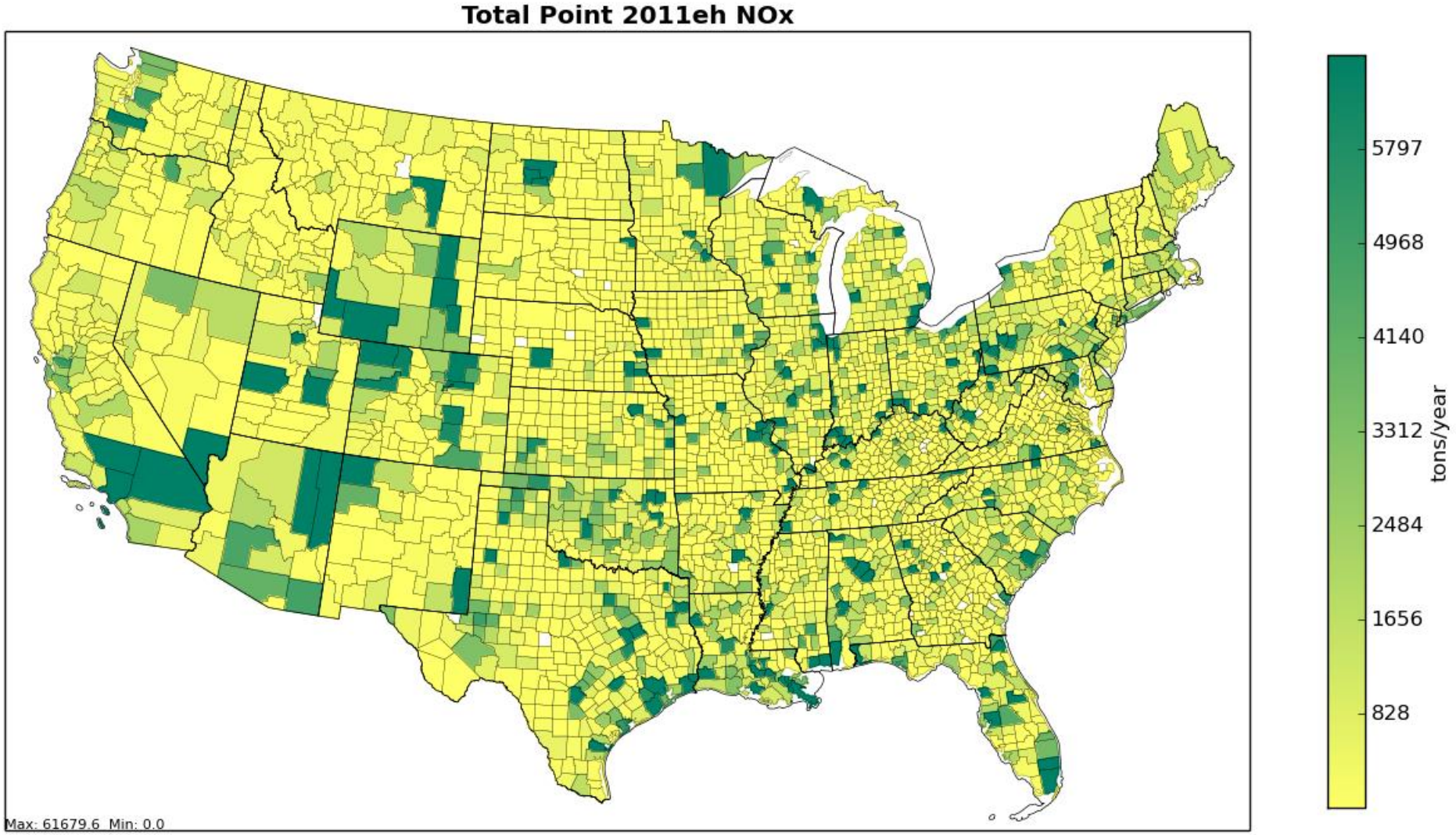
Oil and gas VOC went up due to new processes included; onroad from MOVES

VOC in 2011eh (v2) vs 2011ed (v1)

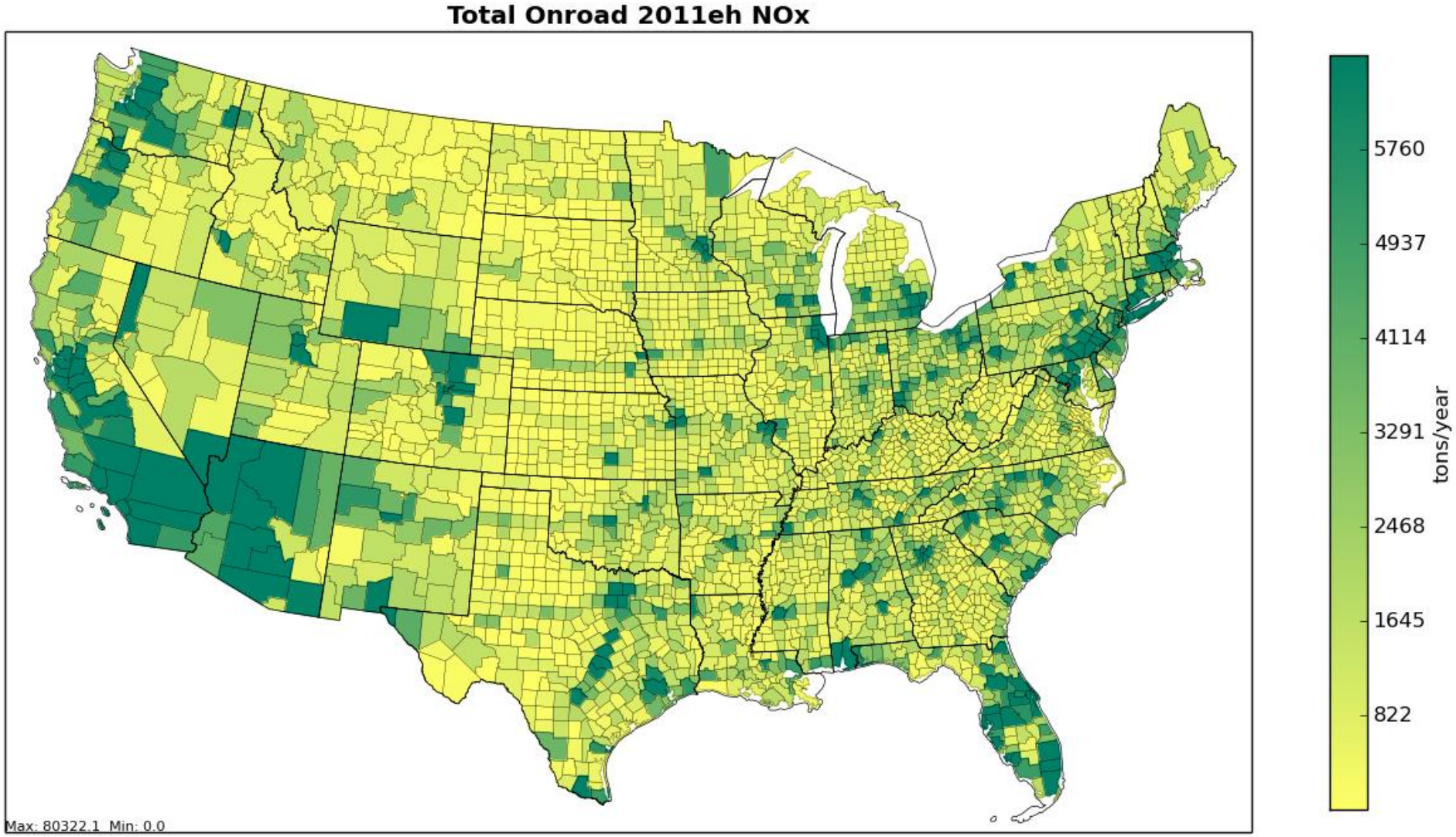


	VOC_INV beis	VOC_INV c1c2rail	VOC_INV c3marine	VOC_INV nonpt	VOC_INV nonroad	VOC_INV np_oilgas	VOC_INV onroad	VOC_INV othar	VOC_INV othon	VOC_INV othpt	VOC_INV pt_oilgas	VOC_INV ptegu	VOC_INV ptnonipm	VOC_INV rwc	VOC_INV ptfire
2011ed	40,648	55,229	5,110	3,792,	2,049,	2,273,	2,445,	1,431,	273,82	329,59	89,754	33,159	872,64	447,59	5,174,
2011eh	40,864	54,663	5,149	3,746,	2,049,	2,556,	2,808,	1,297,	497,78	265,44	164,09	36,337	802,62	443,01	4,688,

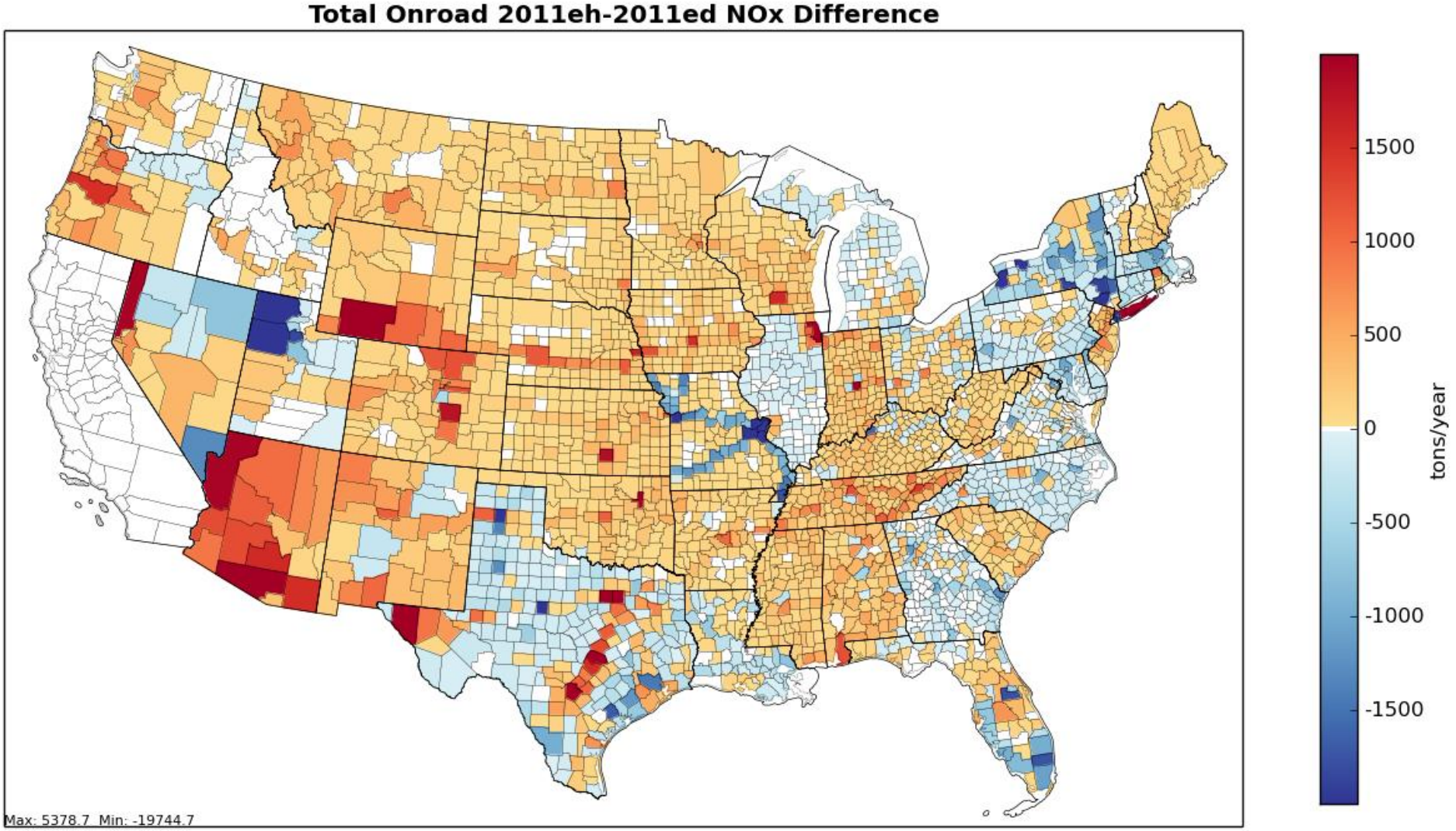
Maps help us see spatial variation and hot spots

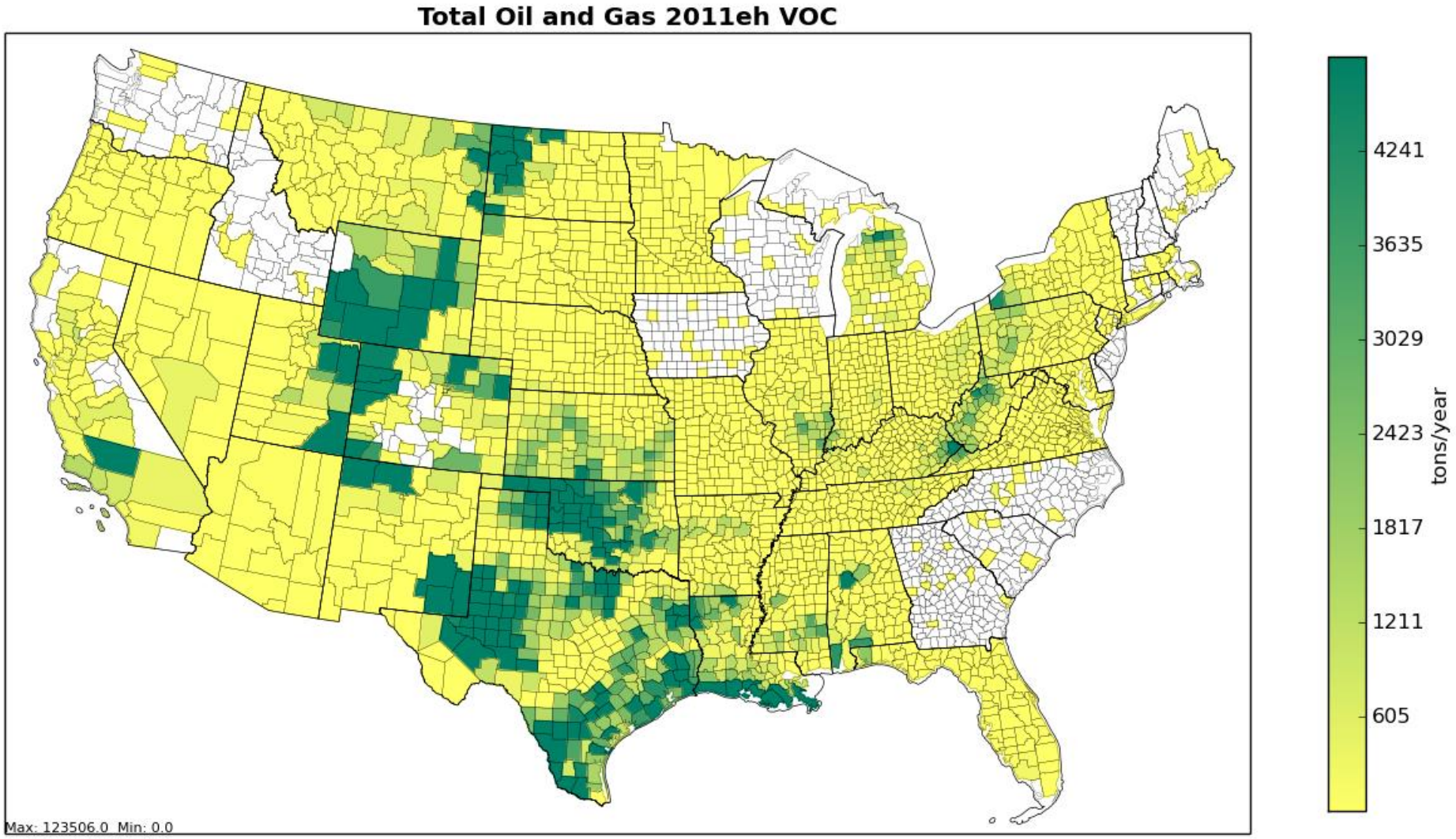


Notice the higher NOx emissions in counties with interstates

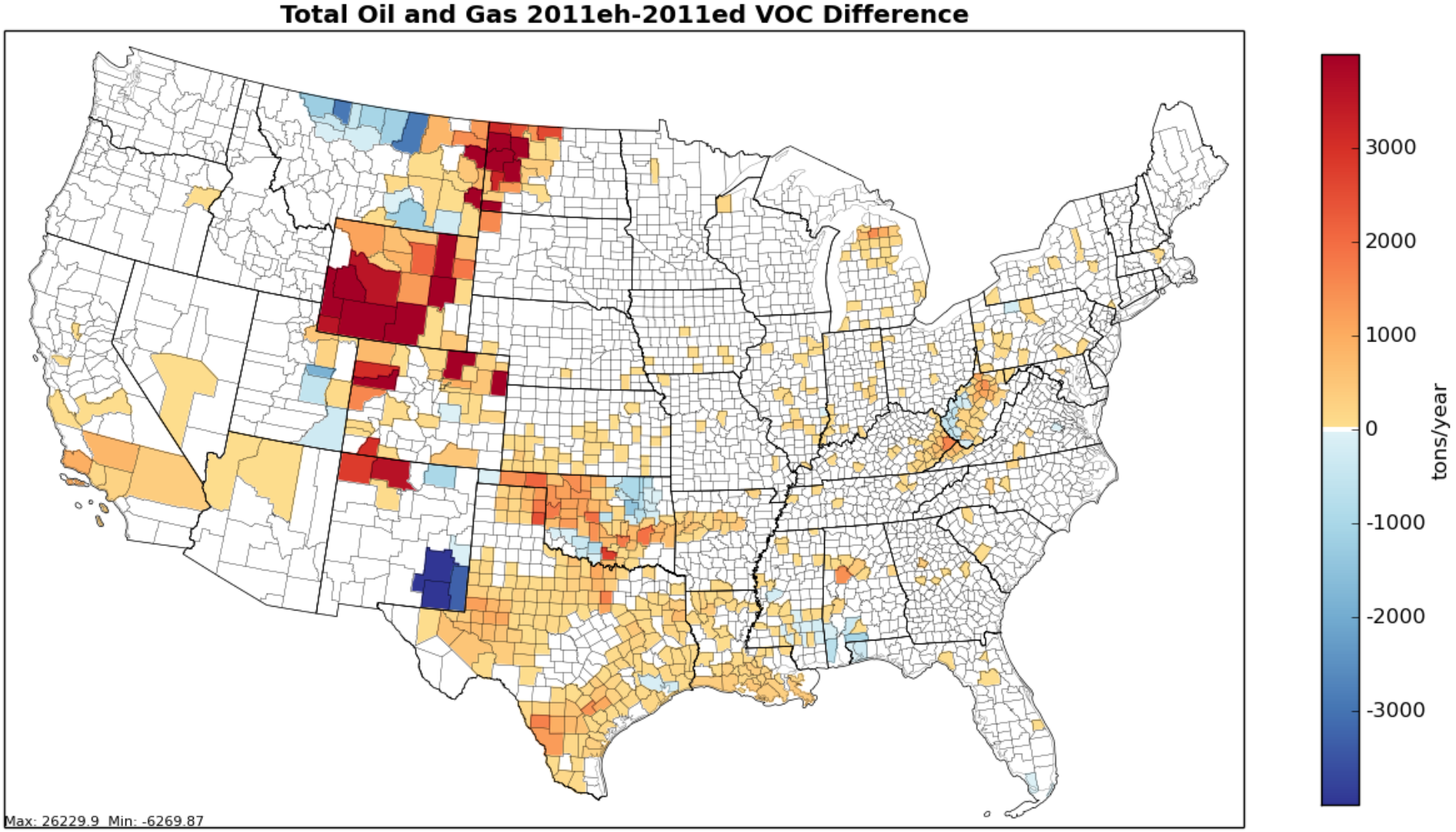


MOVES inputs changed substantially from 2011NEIv1 to 2011NEIv2




Total Oil and Gas 2011eh VOC
Max: 123506.0 Min: 0.0
4241
3635
3029
2423
1817
1211
605
tons/year

Oil and gas VOC increased due to more processes and data resubmissions



Questions?

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

Emissions Modeling with SMOKE

- We use the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system and associated tools to process our emissions into air quality model-ready files
  - Smkinven: reads in the inventories
  - Grdmat: computes gridding matrix
  - Spcmat: computes speciation matrix
  - Elevpoint: Splits ground-level and elevated emissions
  - Temporal: temporally allocates emissions to hours
  - Smkmerge: merges all matrices and temporalized emissions to create AQM-ready data for a sector
  - Movesmrg: merges all matrices, MOVES emission factors and temporalized activity to create AQM-ready data for the onroad sector
  - Mrggrid: merges ground-level emissions together

Emissions Models Used

- **Biogenic Emission Inventory System (BEIS):** creates air quality model-ready biogenic emissions (SMOKE: Normbeis3, Tmpbeis3)
- **Motor Vehicle Emission Simulator (MOVES)**: generates emission factors for onroad mobile sources that can be combined with activity data within SMOKE (Met4moves, Movesmrg)
- **National Mobile Inventory Model (NMIM):** generates inventories for nonroad sources (this function is being folded into MOVES)
- **Integrated Planning Model (IPM):** generates EGU emissions for future year modeling

Other Emissions Modeling Tools

- Surrogate Tool: creates spatial surrogates used for gridding from Shapefiles
- Speciation Tool: creates speciation profiles used for speciation from SPECIATE profiles
- Gentpro: SMOKE program to create meteorology-based temporal profiles
- Emissions Modeling Framework: graphical user interface that manages inventories and related data and modeling cases; creates summaries for QA and analysis; projects inventories with CoST
- Python: helps with QA, creates maps

Emissions Modeling Steps by Sector

Platform sector	Spatial	Speciation	Inventory resolution
afdust	Surrogates	Yes	annual
ag	Surrogates	Yes	annual
agfire	Surrogates	Yes	monthly
beis	Pre-gridded land use	in BEIS 3.6.1	computed hourly
c1c2rail	Surrogates	Yes	annual
c3marine	Surrogates	Yes	annual
nonpt	Surrogates & area-to-point	Yes	annual
nonroad	Surrogates & area-to-point	Yes	monthly
np_oilgas	Surrogates	Yes	annual
onroad	Surrogates	in MOVES 2014	monthly activity, computed hourly
onroad_ca_adj	Surrogates	in MOVES 2014	monthly activity, computed hourly
rwc	Surrogates	Yes	annual

Emissions Modeling Steps (ctd.)

Platform sector	Spatial	Speciation	Inventory resolution	Plume rise
othafdust	Surrogates	Yes	annual	
othar	Surrogates	Yes	annual	
othon	Surrogates	Yes	annual	
othpt	Point	Yes	annual	in-line
pt_oilgas	Point	Yes	annual	in-line
ptegu	Point	Yes	daily & hourly	in-line
ptprescfire	Point	Yes	daily	in-line
ptwildfire	Point	Yes	daily	in-line
ptnonipm	Point	Yes	annual	in-line

Plume Rise

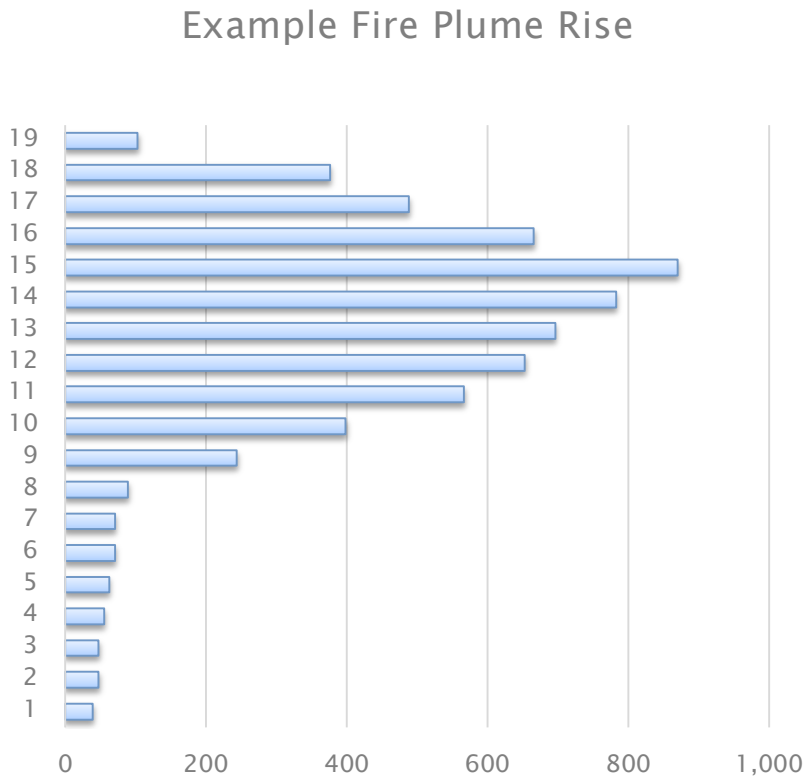
- Plume rise allows for sources to go above the first layer of the air quality model
- The SMOKE Elevpoint program selects elevated or plume-in-grid point sources with Briggs algorithm
  - EPA uses the cut-off method to treat sources with approximate plume height over 20m as elevated
- **Stack parameters** for point sources affect plume rise
- Plume rise can be done with the SMOKE Laypoint program to compute layer fractions for each elevated point source

  * **A special plume rise treatment is used for fires that is a function of acres burned and heat flux**
- CMAQ can do "in-line" plume rise so that only 2-D hourly emissions plus information about locations and emissions for elevated sources can be provided (3-D emissions are really big!)

Plume Rise Formula

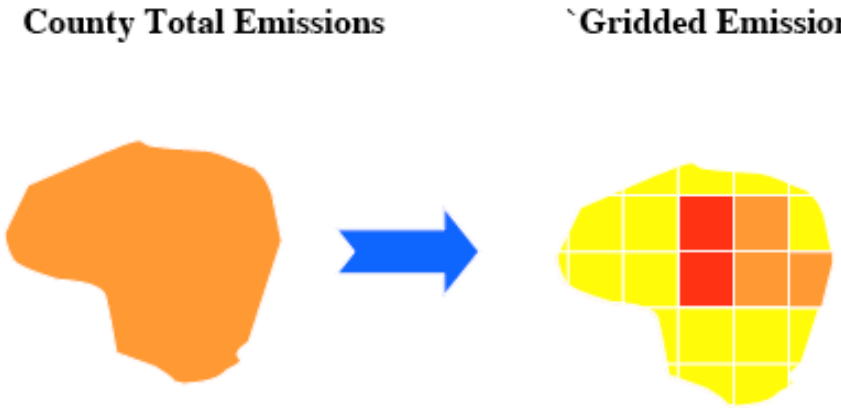
- $F = 0.25 \times G \times V_S \times D_S^2 \times (T_S - T)/T_S$
- For F less than 55,
  Plume rise $= H_S + 21.31311057 \times F^{0.75}/U$
  otherwise:
  Plume rise $= H_S + 38.87776061 \times F^{0.6}/U$ where
  - F = Bouyancy flux (m^4/s^3)
  - G = Mean gravitational acceleration (9.80665 m/s^2)
  - V_S = Stack gas exit velocity (m/s)
  - D_S = Inside stack diameter (m)
  - T_S = Stack gas temperature (K)
  - T = Default ambient air temperature (293 K)
  - U = Default wind speed (2 m/s)
  - H_S = Physical stack height (m)

Allocation to Layers for AQ Modeling



Spatial Allocation

- Process of mapping inventory emissions to modeling grid cells
- There are many types of surrogates, and each has a unique code
  - Typically use SCC to X-ref surrogate to inventory
  - Population (100), Total agriculture (310), Railroad Density (271), Offshore shipping (806), Urban unrestricted roads (221), Gas well count (698)

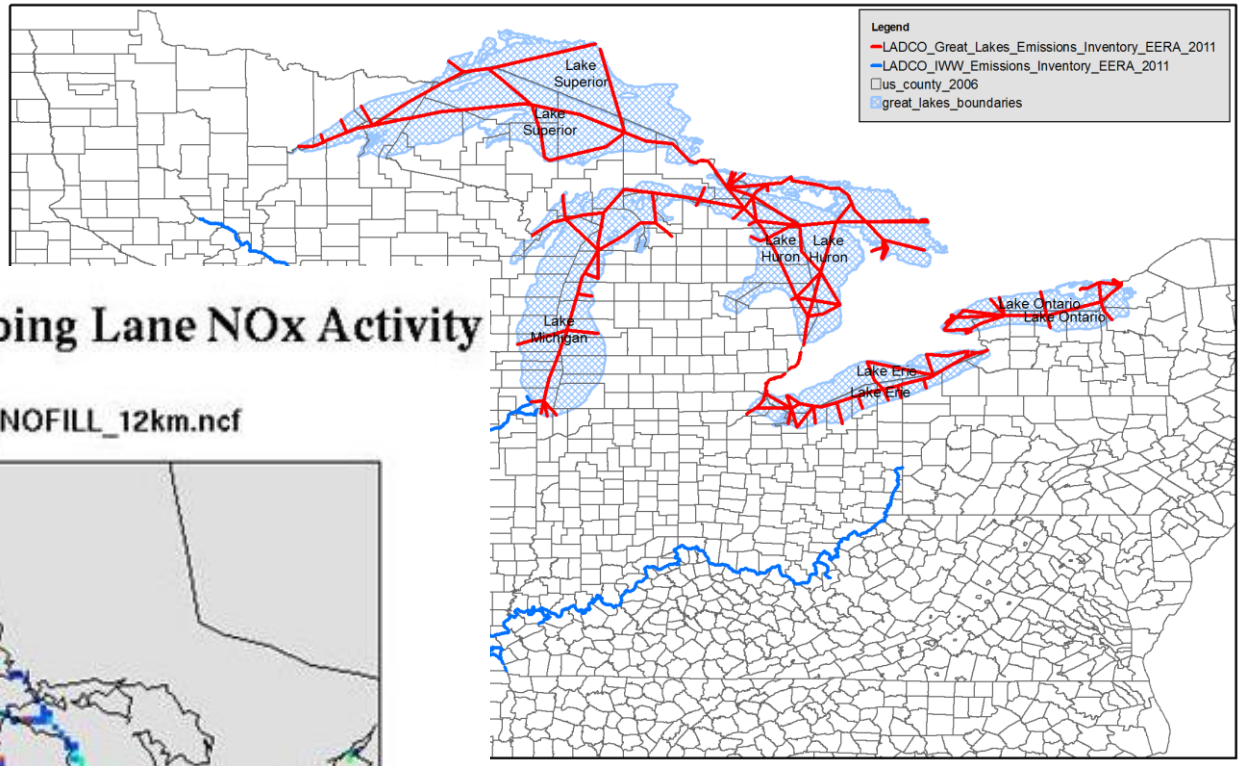


Data Used to Create a Spatial Surrogate with Surrogate Tool

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

Creating a Great Lakes Surrogate

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



Spatial Surrogate values

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

Sum to 1 for each county / province

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

Using Cross-references and Profiles (Generically)

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

X-REF table

County, ID	
Durham,NC	15
Orange,NC	15
Wake,NC	16
SC, All	17

Profiles table (sum to 1)

ID, Factor 1, 2, 3	
13	0.2, 0.3, 0.5
14	0.4, 0.4, 0.2
15	0.4, 0.3, 0.3
16	0.4, 0.5, 0.1
17	0.4, 0.4, 0.2

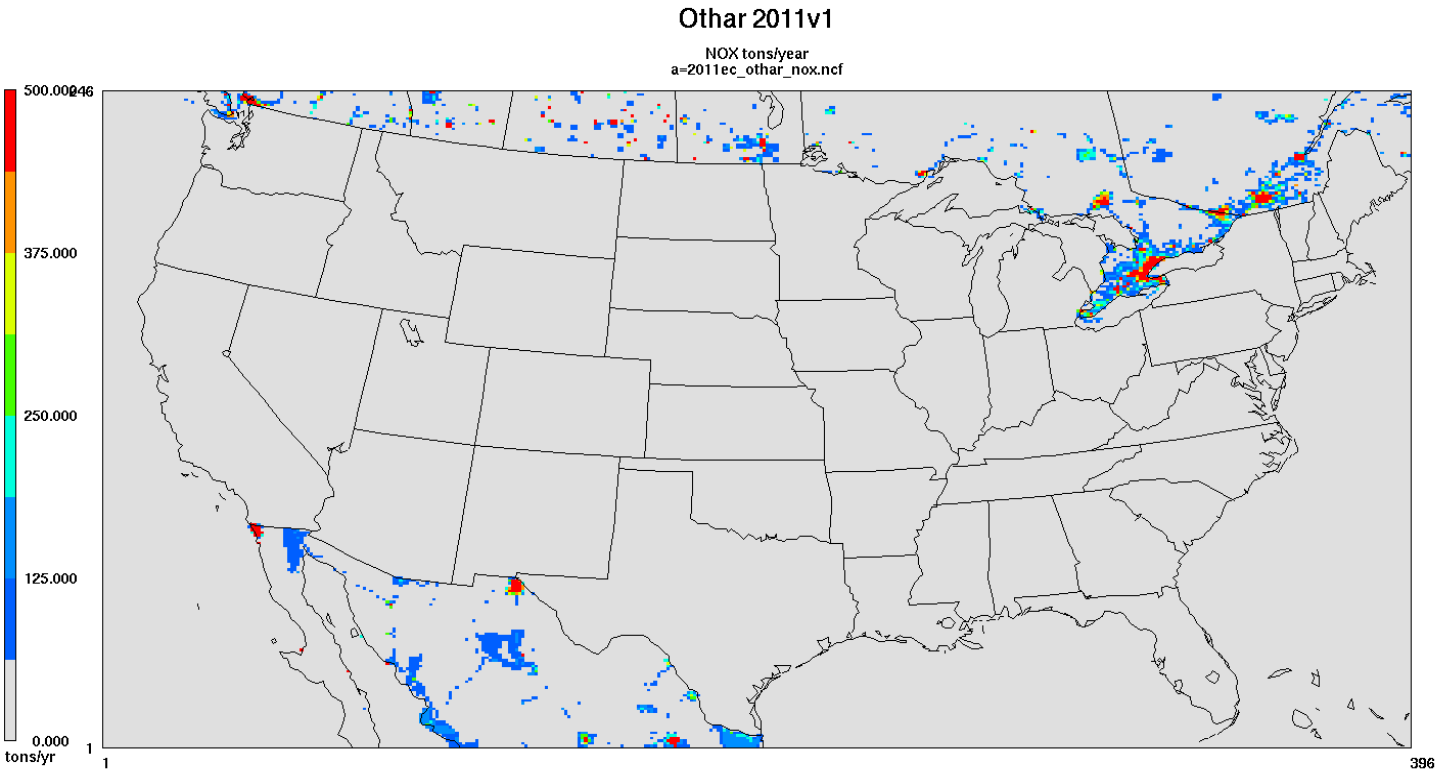
Spatial Surrogate Cross reference

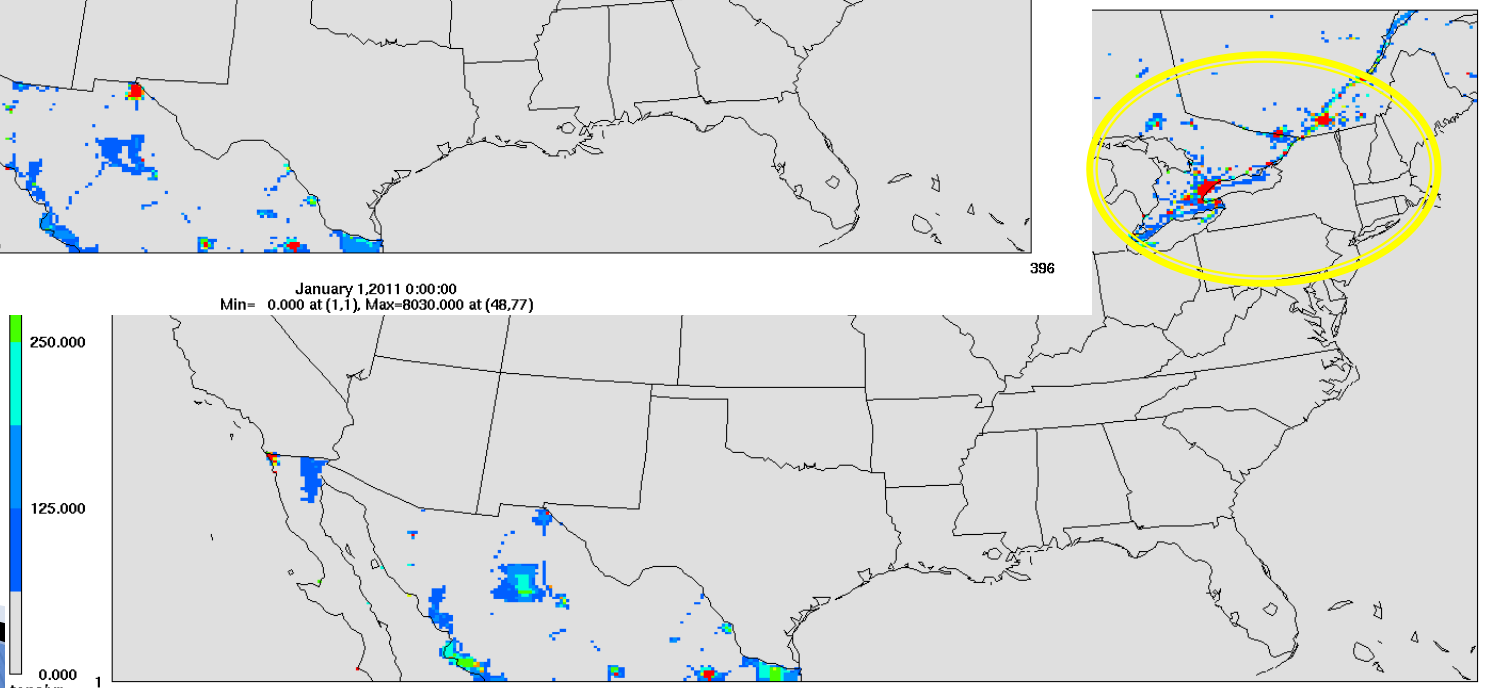
FIPS ST/CTY	SCC	Surrogate ID	Comments
000000	0040600241	801	! All counties
000000	0040600242	801	! All counties
000000	2505020121	801	! All counties
048243	20100102	693	! Replaced 698
048243	20200201	693	! Replaced 698
008001	20100102	689	

Quality Assurance of Spatial Allocation

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

QA of Non US Spatial Allocation

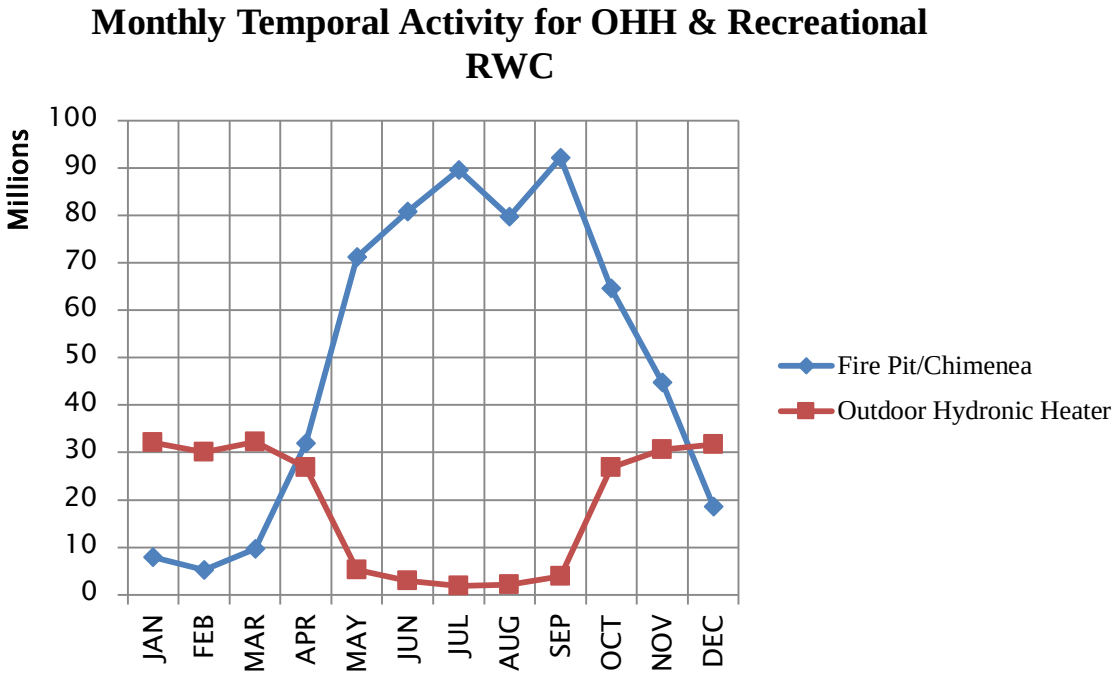


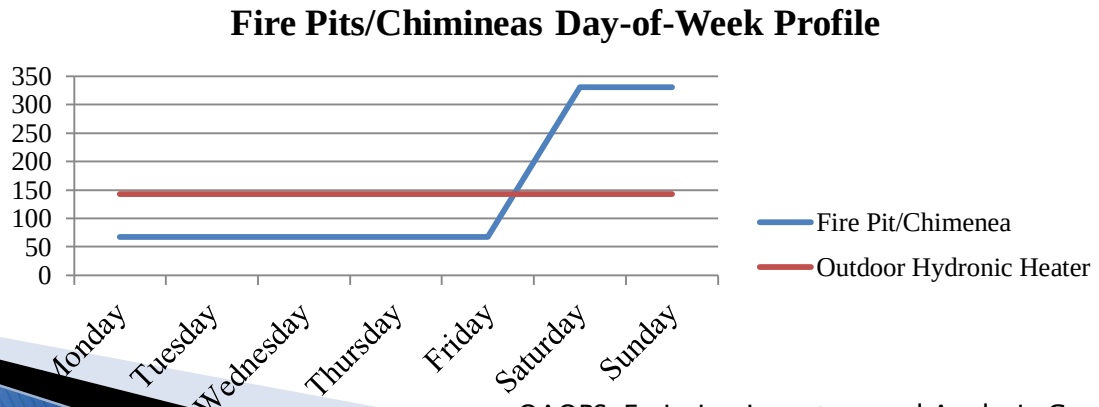


Temporal Allocation

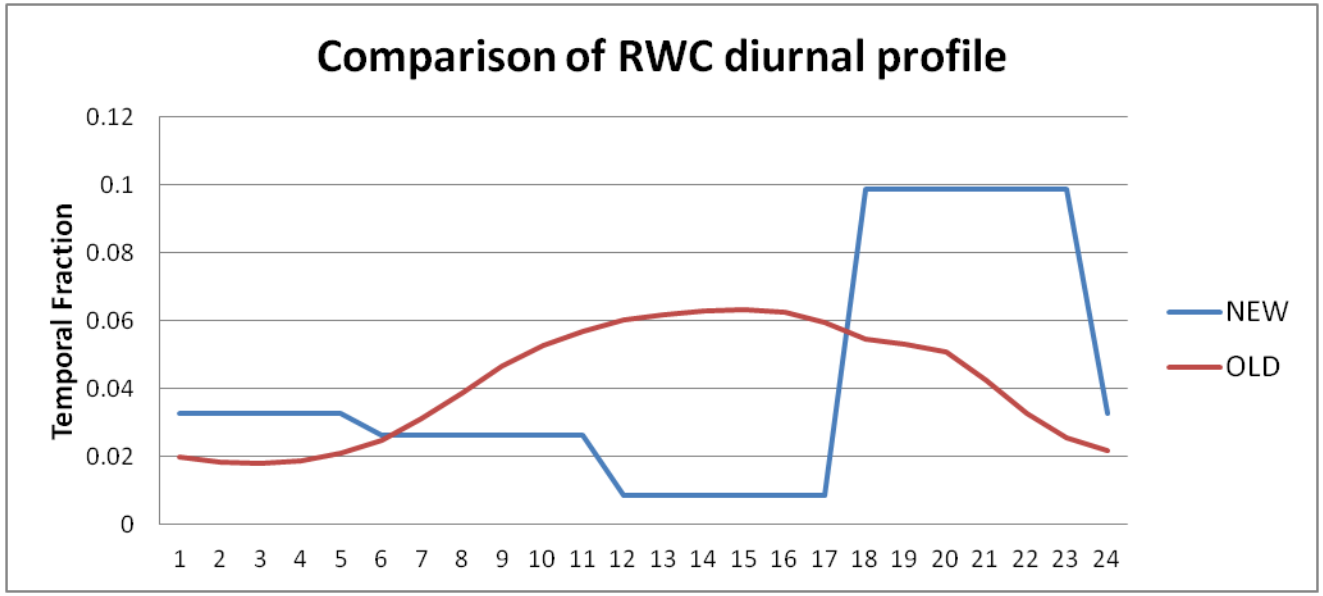
- Process of allocating inventory emissions to modeling hour emissions
- Hierarchy of temporalization steps: annual -> month -> day -> hour
- There are many types of temporal profiles for each resolution and each has a unique code
  - Typically use SCC to map temporal profiles to inventory sources
  - Also may use FIPS, pollutant, etc. in cross reference
- More control with the new format in SMOKE 3.6
  - e.g., Monday diurnal profile vs Friday diurnal profile
  - Database friendly

Temporal Profile Examples (1 of 2)





Temporal Profile Examples (2 of 2)



Excerpt from Temporal Cross Reference and Profile Files

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

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

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

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

Temporal Settings by Sector

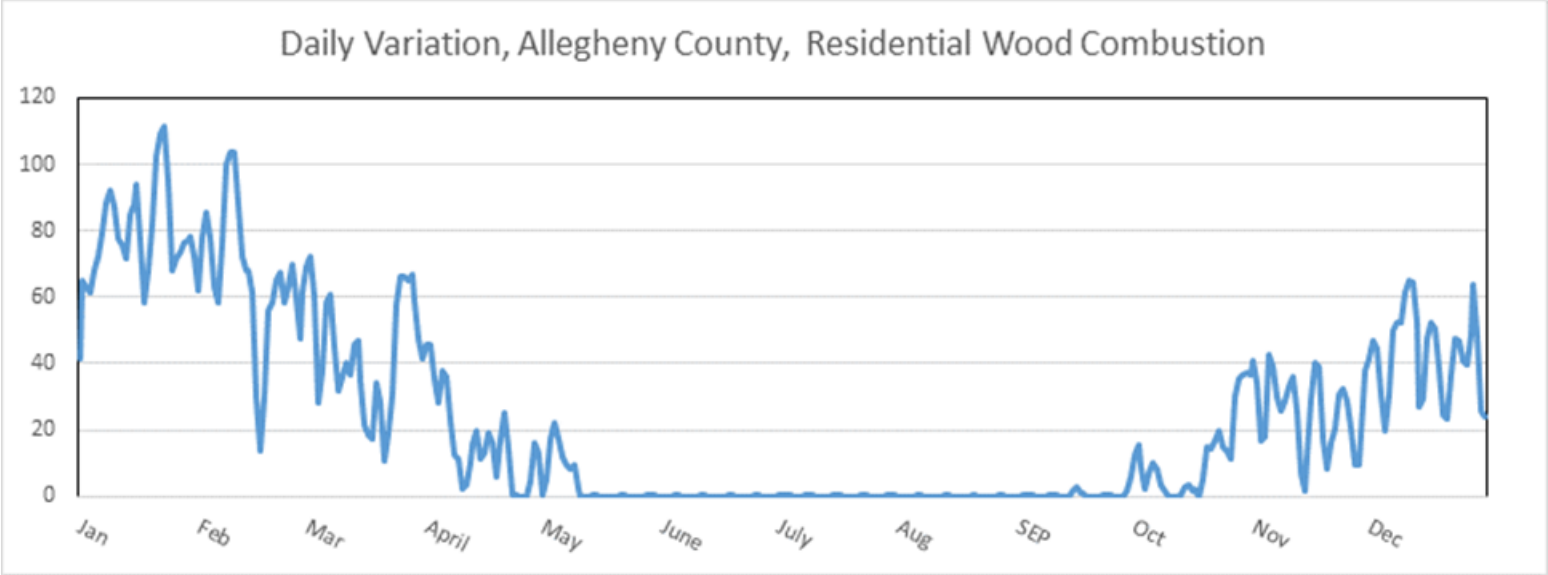
Platform sector short name	Inventory resolutions	Monthly profiles used?	Daily temporal approach	Merge processing approach	Process Holidays as separate days?
afdust_adj	Annual	yes	week	all	Yes
ag	Annual	yes	all	all	Yes
agfire	Monthly		week	week	Yes
beis	Hourly		n/a	all	Yes
c1c2rail	Annual	yes	mwdss	mwdss	
c3marine	Annual	yes	aveday	aveday	
nonpt	Annual	yes	week	week	Yes
nonroad	Monthly		mwdss	mwdss	Yes
np_oilgas	Annual	yes	mwdss	mwdss	Yes
onroad	Annual & monthly[1]		all	all	Yes
onroad_ca_adj	Annual & monthly[1]		all	all	Yes
othar	Annual	yes	week	week	
othon	Annual	yes	week	week	
othpt	Annual	yes	mwdss	mwdss	
pt_oilgas	Annual	yes	mwdss	mwdss	Yes
ptegu	Daily & hourly		all	all	Yes
ptnonipm	Annual	yes	mwdss	mwdss	Yes
ptprescfire	Daily		all	all	Yes
ptwildfire	Daily		all	all	Yes
rwc	Annual	no	met-based	all	Yes

Meteorology-based Temporalization

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

GenTPRO: rwc

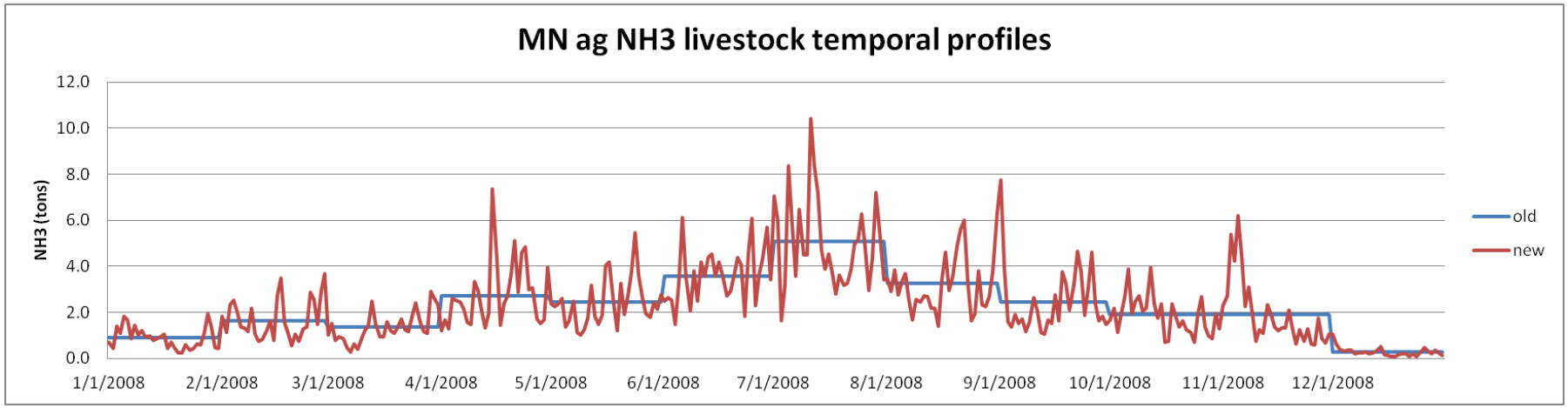
- Meteorological fields: temperature
- annual -> day profile



Note in summer RWC near 0

GenTPRO: ag livestock

- Meteorological fields: temperature, wind speed, and aerodynamic resistance
- month-> hour profile

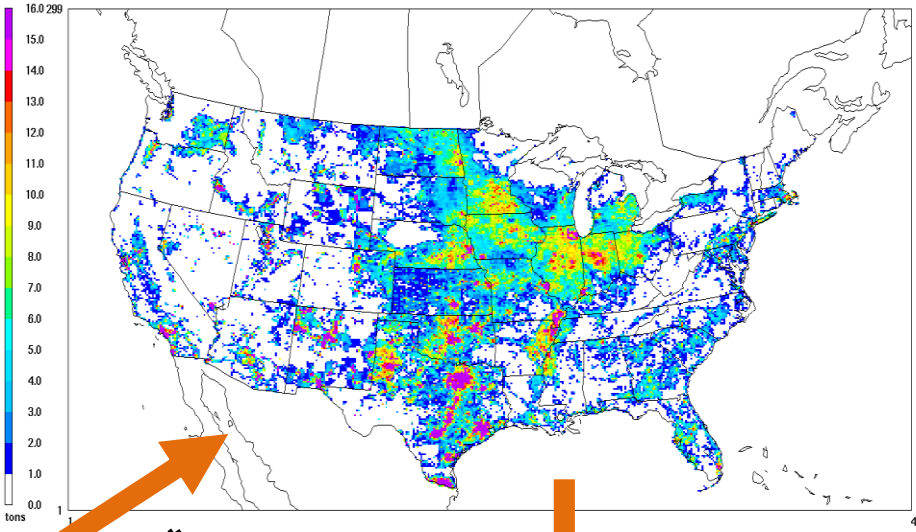


QA of Temporal Allocation

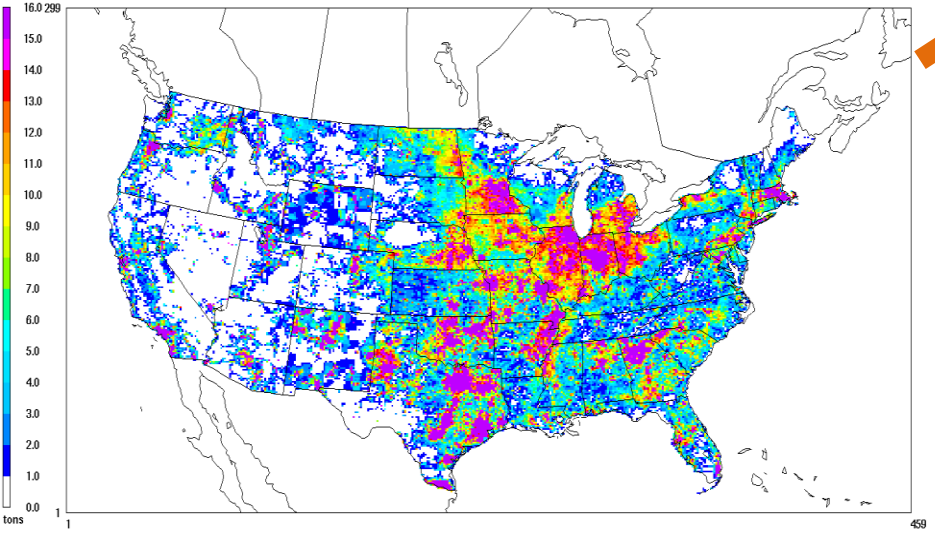
- Check SMOKE temporal logs to ensure all sources have reference to temporal profiles
- Sum post-SMOKE daily emissions by sector to compare back to annual for inventory comparison
- Perform various specialized analysis of EGUs (partial year reporters, spikes in CEMs data)
- Check the PTSUP files to confirm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

Afdust

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

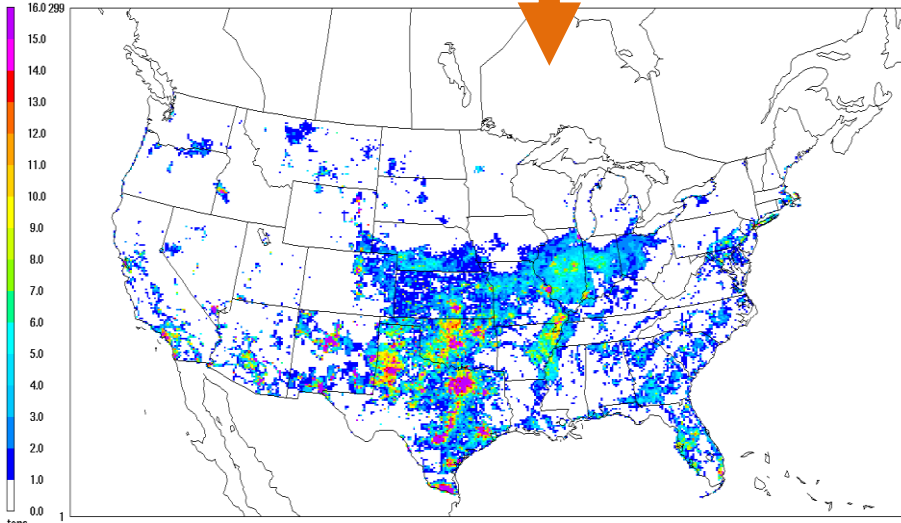


Transport



Unadjusted

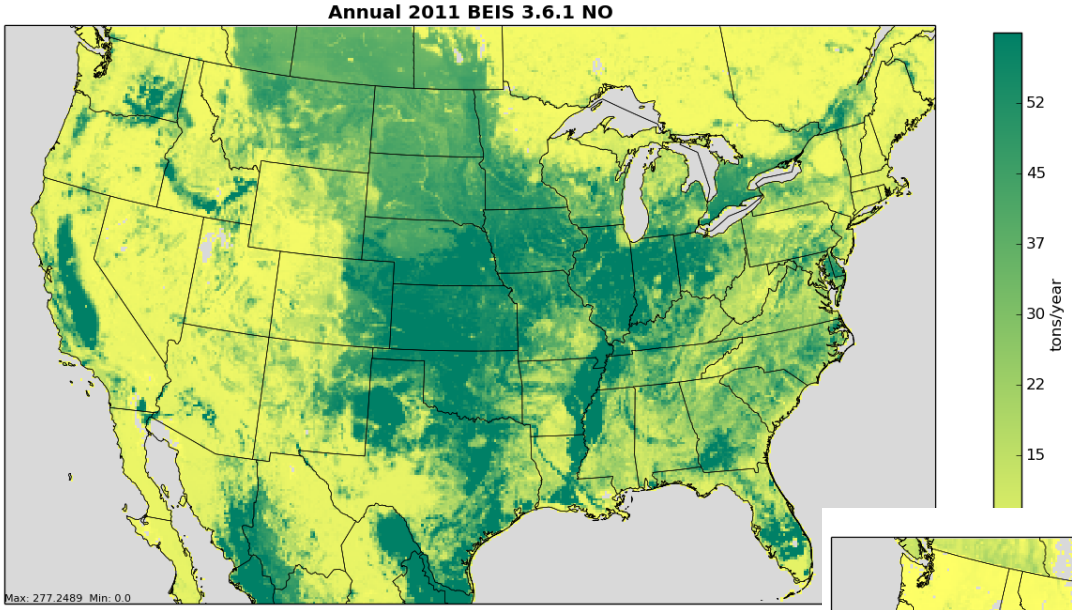
Precipitation

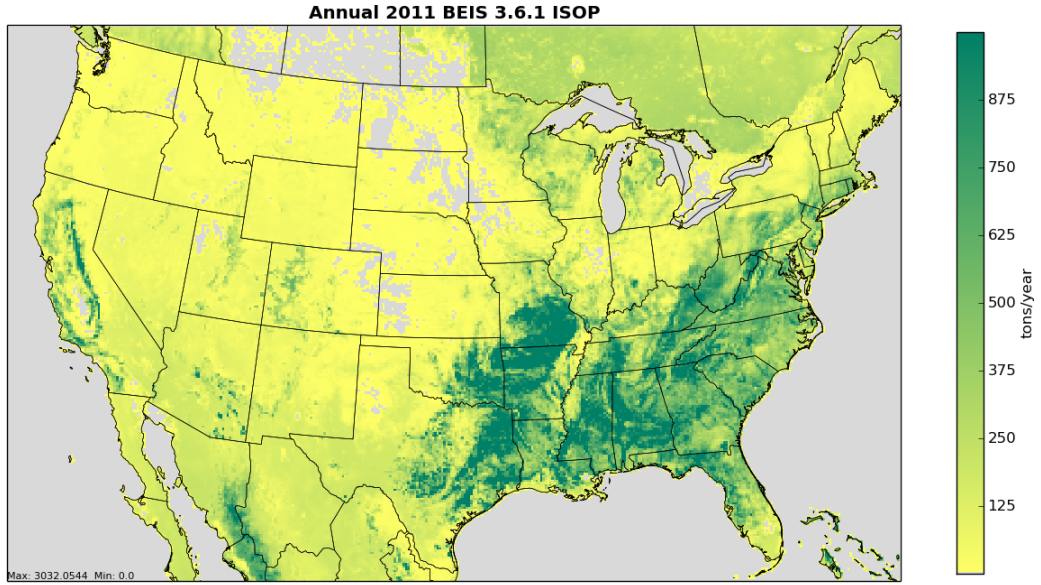


BEIS 3.6.1: Updated Biogenic Emissions

- Updated leaf temperature algorithm
  - Leaf temperature calculated using canopy model rather than 2 meter temperature
- Land use based on:
  - U.S. National Land Cover Database (NLCD) 2006
  - Moderate Resolution Imaging Spectroradiometer (MODIS) for Canada and Mexico
  - Forest areas constrained by canopy coverage
- Tree species from USFS Forest Inventory and Analysis (FIA) data v5.1
  - Selected surveys from 2002 to 2012 to get a complete decadal US survey that bounds the years being modeled
- SMOKE programs:
  - Normbeis3: normalized biogenic emissions
  - Tmpbies3: outputs gridded, speciated, hourly emissions

Annual Biogenic Emissions

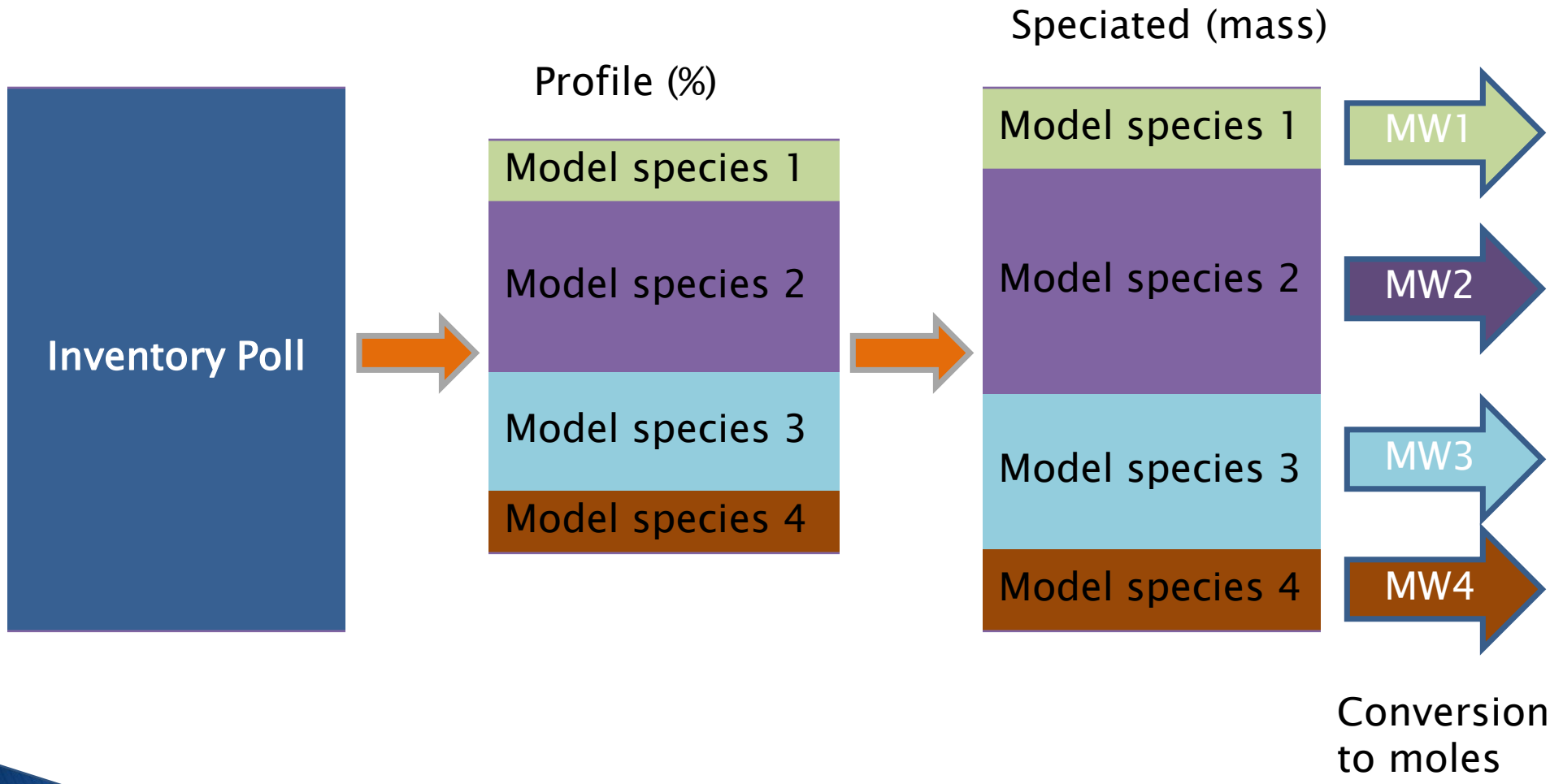




Speciation

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

Speciation Overview



NOx Speciation

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

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

$PM_{2.5}$ Speciation

- Previous versions of CMAQ had "simplified" PM model species (AE5)
- Latest version of CMAQ has a new 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 (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

- TOG factors
  - Inventory VOC is typically converted to TOG (Total Organic Gas)
  - Example for Gas Exh E10: VOC * 1.199 = TOG
- Chemical mechanism specific:
  - Different model species depending on the chemical mechanism
  - CB05 example:

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

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

Gasoline Exhaust – E10 (8751a)

VOC Integration (1 of 3)

- Integration
  - Process of taking select VOC HAPs from the inventory and speciating the remaining VOC
  - Want to avoid double counting
  - Want to speciate the remaining VOC taking into account HAPs that were removed
- BAFM
  - Benzene, Acetaldehyde, Formaldehyde, Methanol
  - List of explicit VOC HAPs
- NONHAPVOC
  - Remaining VOC after remove explicit VOC HAPs
  - NONHAPVOC = VOC - BAFM
- EBAFM
  - Integration of Ethanol + BAFM
  - Typically for mobile related emissions
  - Need to differentiate the profile numbers to indicate whether BAFM or EBAFM integration (E-profiles)

VOC Integration (2 of 3)

No integrate

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

Gasoline Exhaust – E10 (8751a)

Integrate

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

VOC Integration (3 of 3)

Platform Sector	Approach for Integrating
ptegu	No integration
ptnonipm	No integration
ptfire	No integration
othafdust	No integration
othar	No integration
othon	No integration
ag	N/A – sector contains no VOC
afdust	N/A – sector contains no VOC
biog	N/A – contains specific VOC model species
nonpt	Partial integration (BAFM; EBAFM for future year PFC)
np_oilgas	Partial integration (BAFM)
pt_oilgas	Partial integration (BAFM)
rwc	Partial integration (BAFM)
nonroad	Partial integration (BAFM)
c1c2rail	Partial integration (BAFM)
othpt	Partial integration (BAFM)
c3marine	Partial integration (BAFM)
onroad	Full integration (calculated in the MOVES2014 model)*
onroad_ca_adj	Full integration (calculated in the MOVES2014 model)*

Additional Speciaton Concepts

- COMBO files
  - Method of combining 2 or more speciation profiles by pollutant/geography
  - Example: combine E0 and E10 fuel profiles for PFC
- Speciation can be used to group/track interrelated pollutants
  - PAH's for NATA

Onroad speciaton

- MOVES2014 doing most of speciation within MOVES
  - Different profiles for different vehicle model years, regulatory classes, fuel types, and emission processes
  - Previously used COMBO files or weighted profiles to approximate, but was a coarse approach
  - Can do an explicit mapping of profiles to sources if do speciation within MOVES
- PM2.5
  - AE6 species coming directly from MOVES (in mass)
- VOC
  - 16 pollutants are explicit, i.e. integrated
  - Model species (moles) and inventory pollutants (mass) come directly from MOVES
  - Need to specify chemical mechanism in the MOVES run

QA of Speciation

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

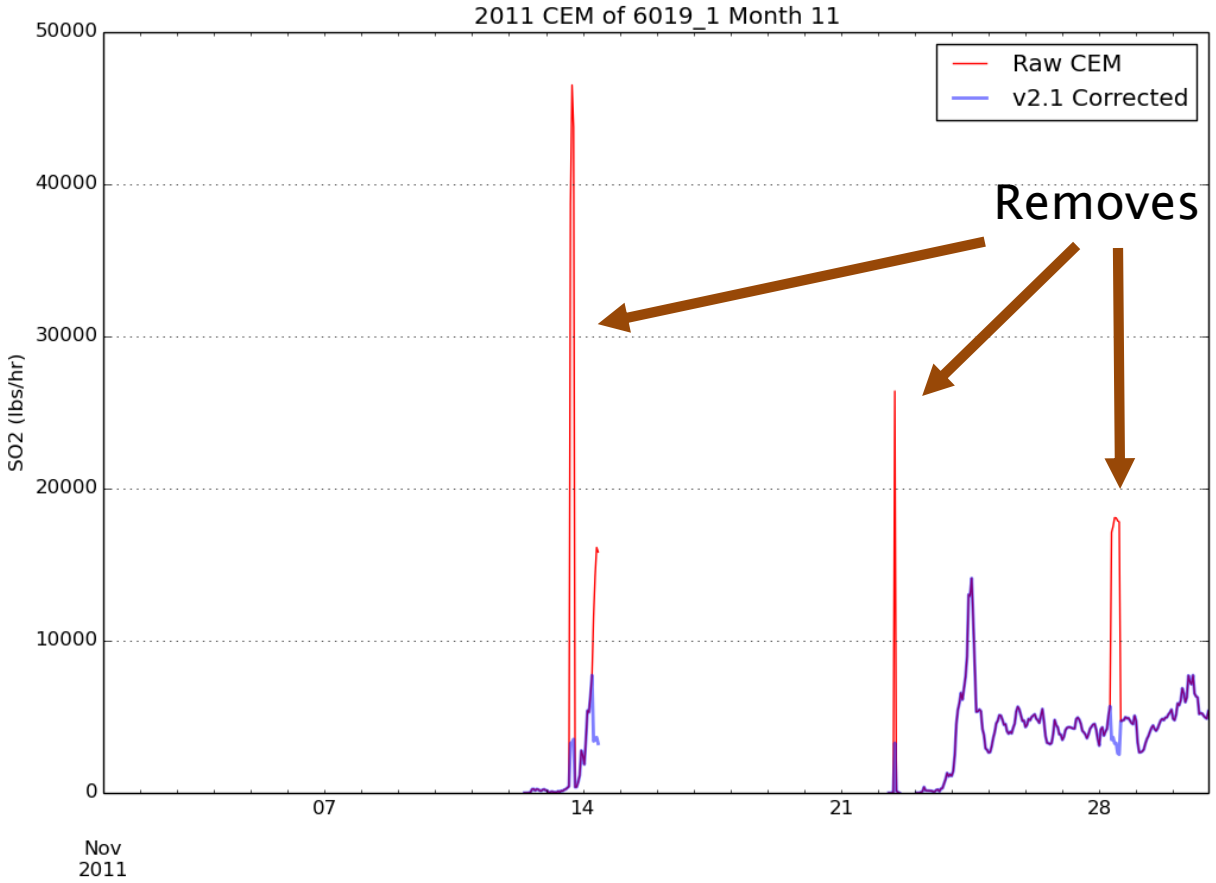
Questions?

- Any questions on spatial gridding, temporalization, or speciation?

Special Steps for EGU Processing

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

Outputs from UNC's CEMS Data Correction Tool



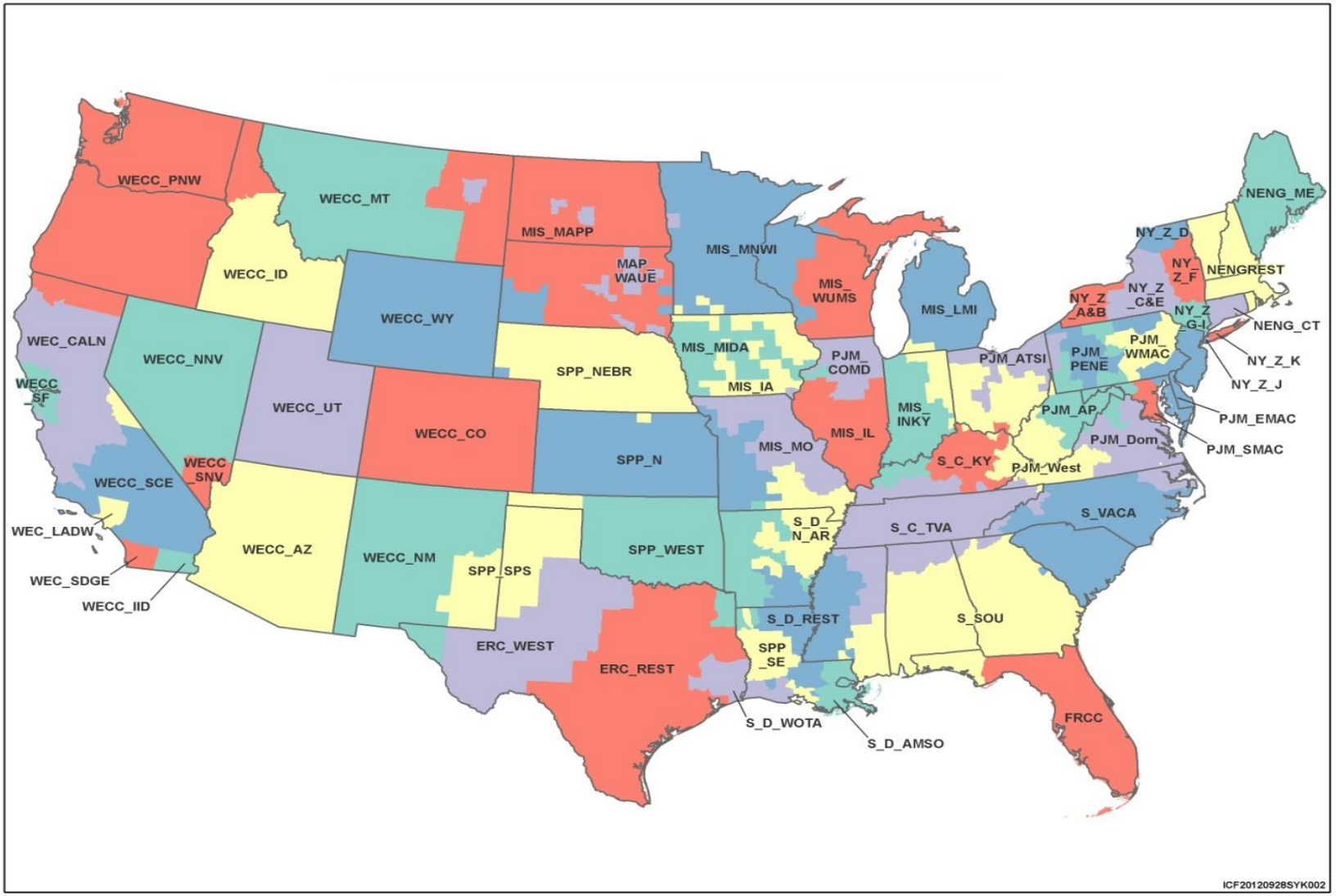
Removes spikes

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

EGU Temporal Profiles and Matching

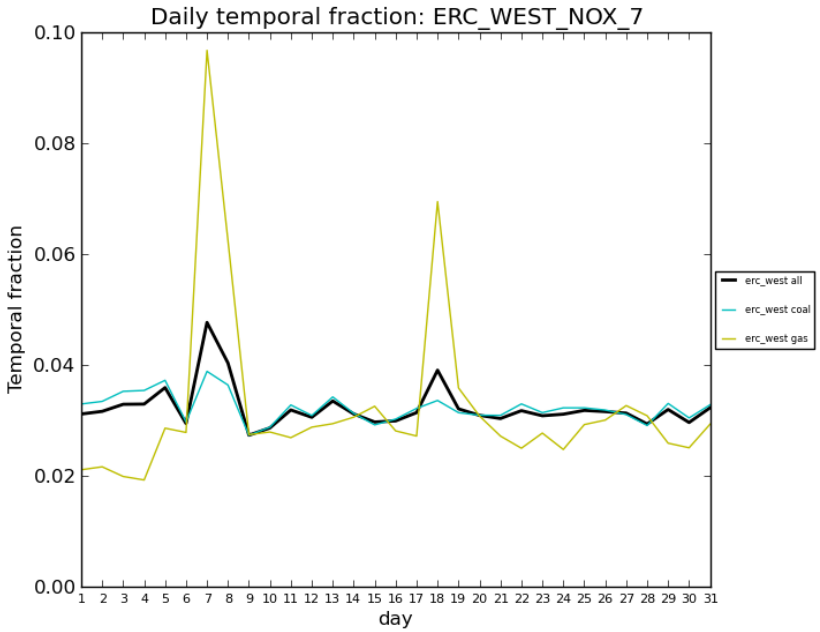
- Removed non-measured data values from CEMS data to ignore emission spikes
- Hierarchy of CEMS assignments:
  1. Use CEMS for all months (units with complete CEMS data)
  2. Use CEMS for months where have measurements, use regional averages for period without measurements (partial-year reporters)
  3. Use regional averages (units without CEMS)
- Regional average profiles
  - IPM region- and fuel-specific average profiles
  - Different winter and summer versions of average hourly profiles
- Extensive additional matching of CEMS database units and IPM units with EIS/platform point sources
  - Mark Janssen led state review; also used for ERTAC model; results fed to CAMD for IPM matching / cross reference

Map of IPM regions

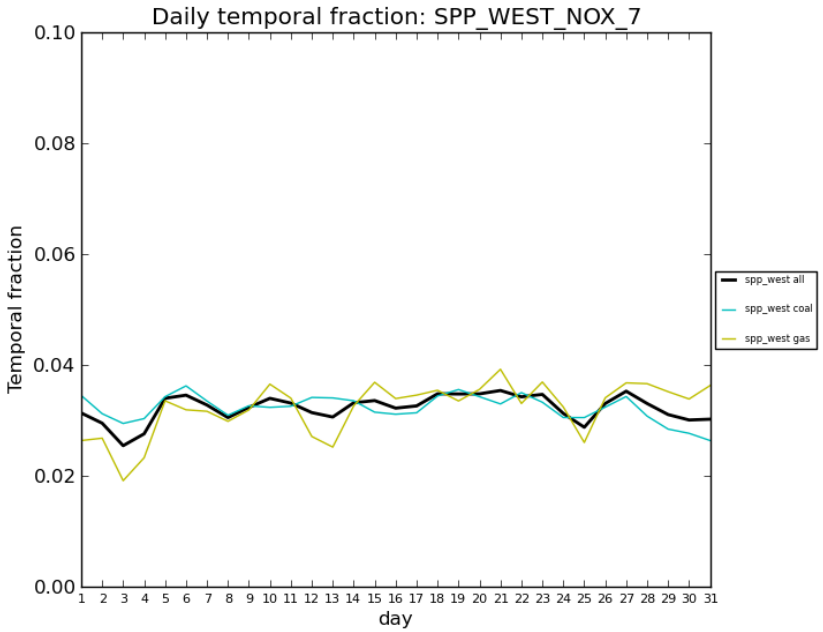


Average Profiles: Region specific

- IPM region- and fuel-specific profiles

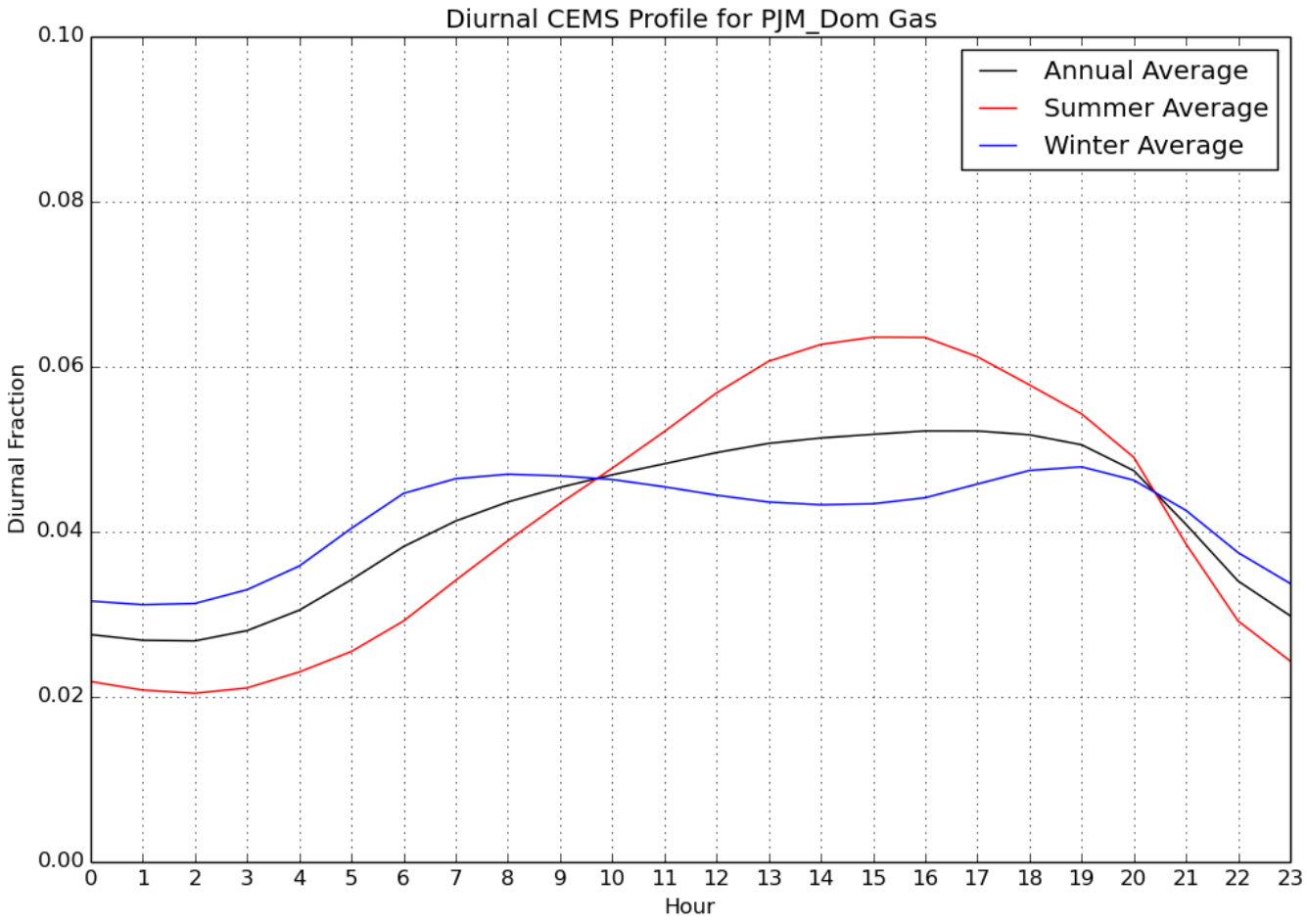


IPM Region in W Texas



IPM Region in E Oklahoma and W Arkansas

Average Profiles: Winter vs. Summer

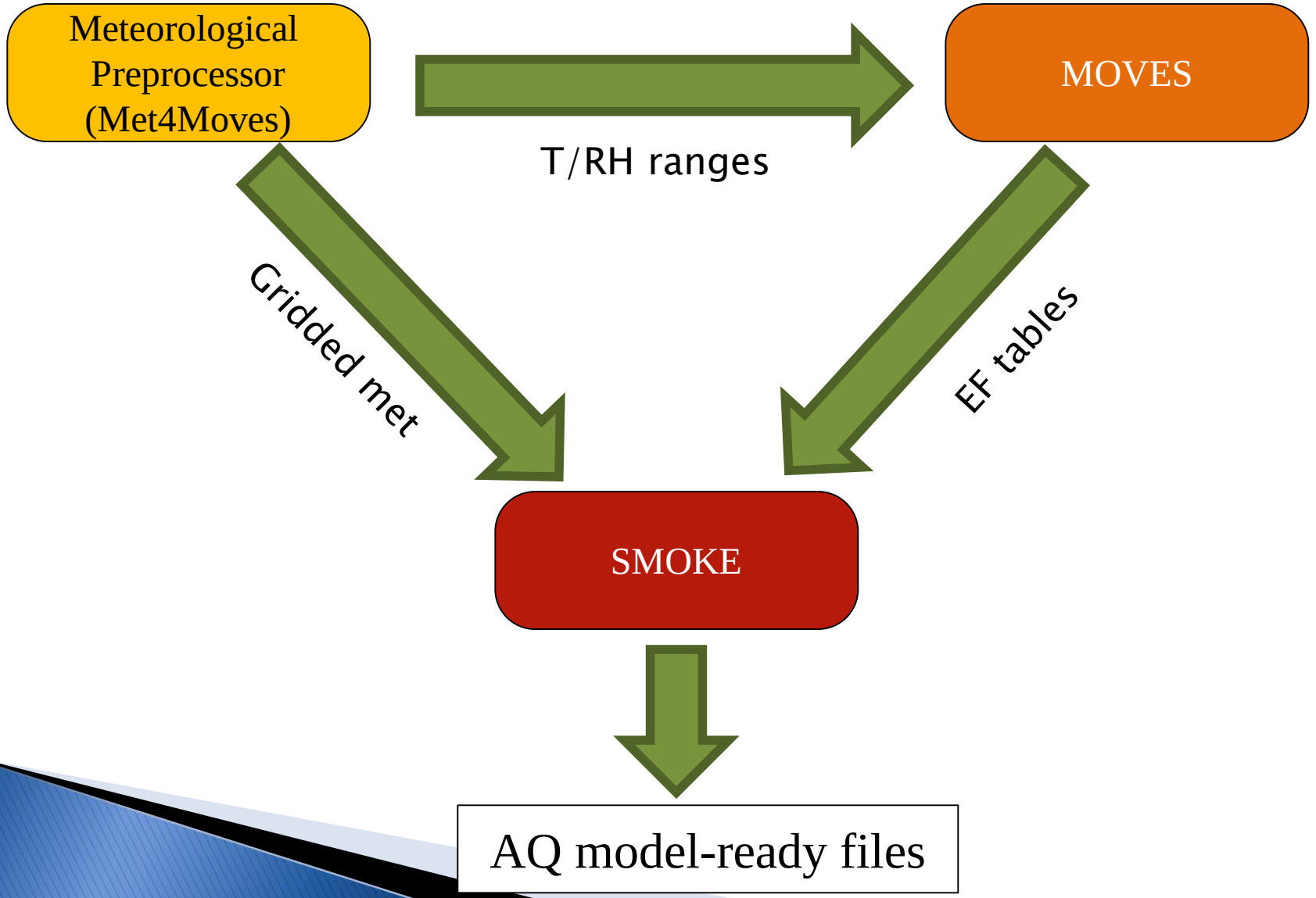


IPM region- and fuel-specific profile

Questions?

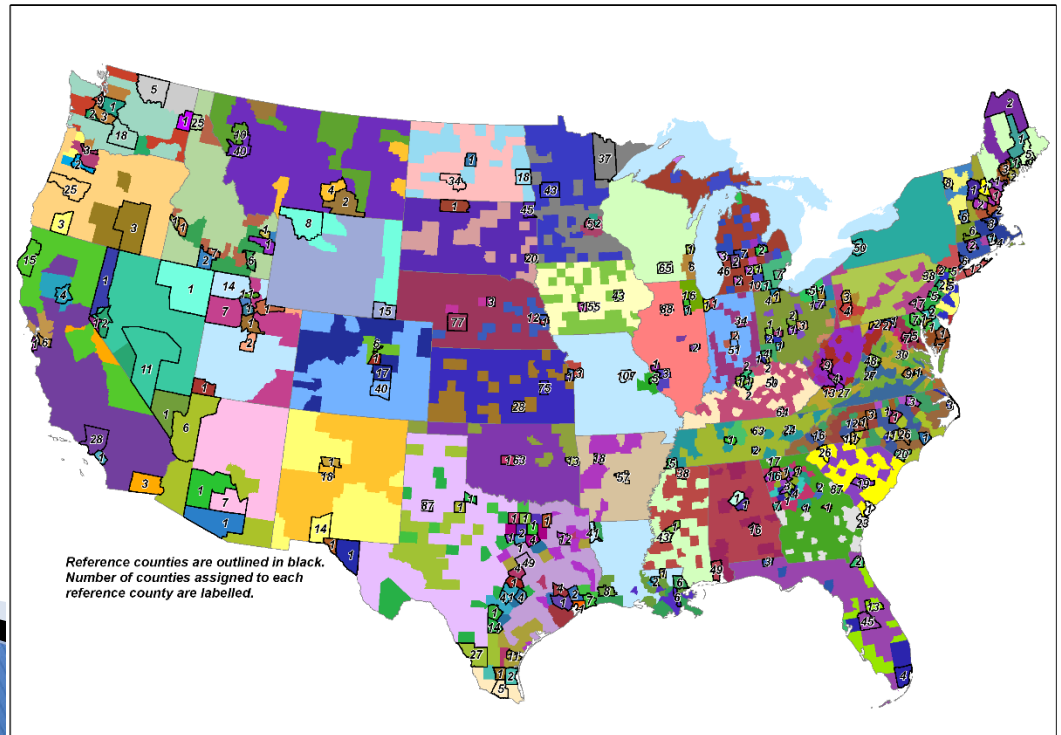
- Any questions on EGU emissions processing?

Onroad Emissions Modeling



Representative Counties

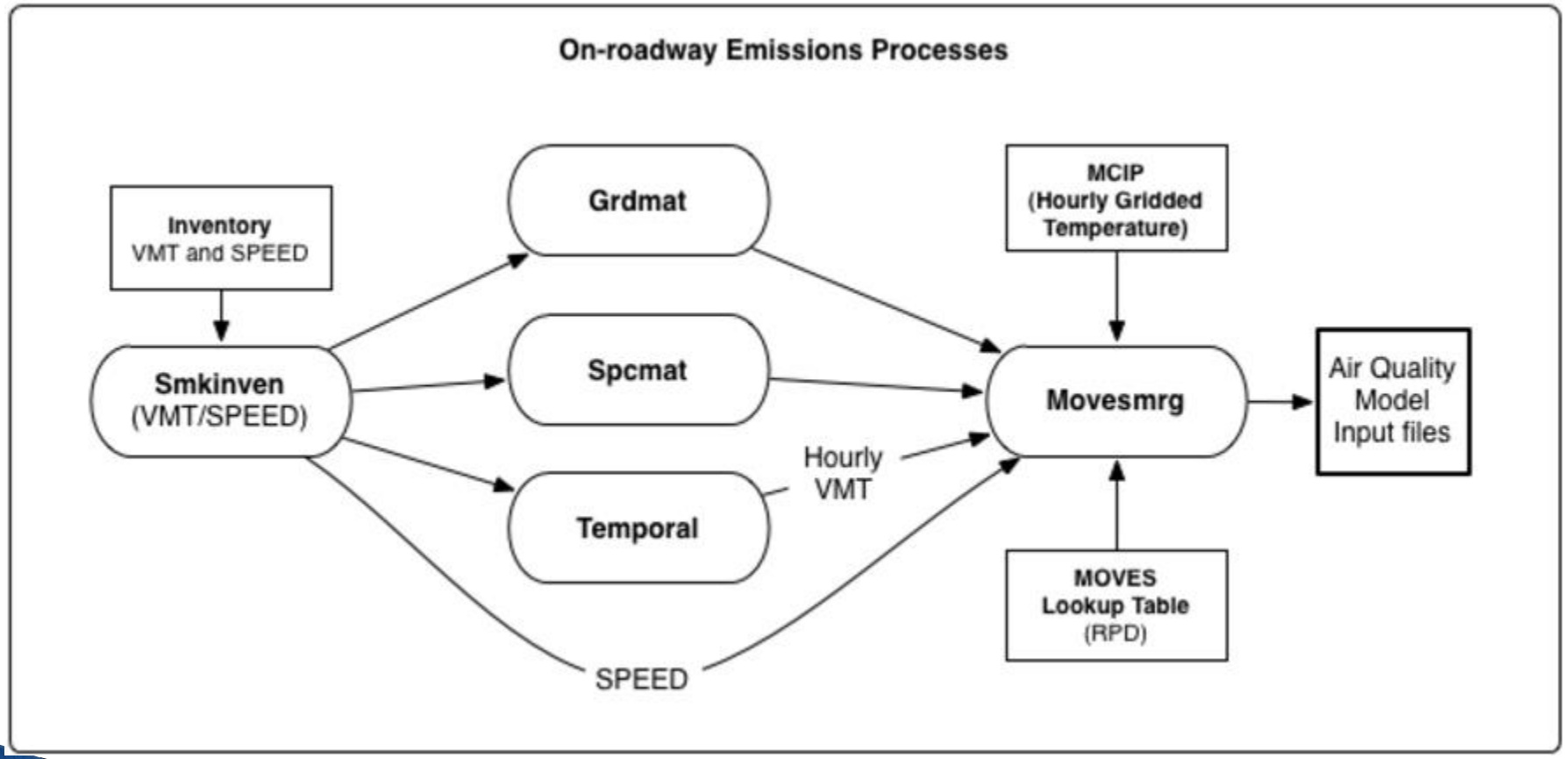
- Map the representative counties to similar counties by:
  - Fuels, age distribution, ramp fraction, I/M program, emissions standards, state
- Run MOVES to get emission factors (EF) for representative counties with detailed: age distribution, fuels, etc.
- Use representative EF and county/grid specific activity and meteorology to create national coverage (via SMOKE)



Emission Processes

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

On-roadway Process (RPD)



Recent Onroad Emissions Modeling Developments

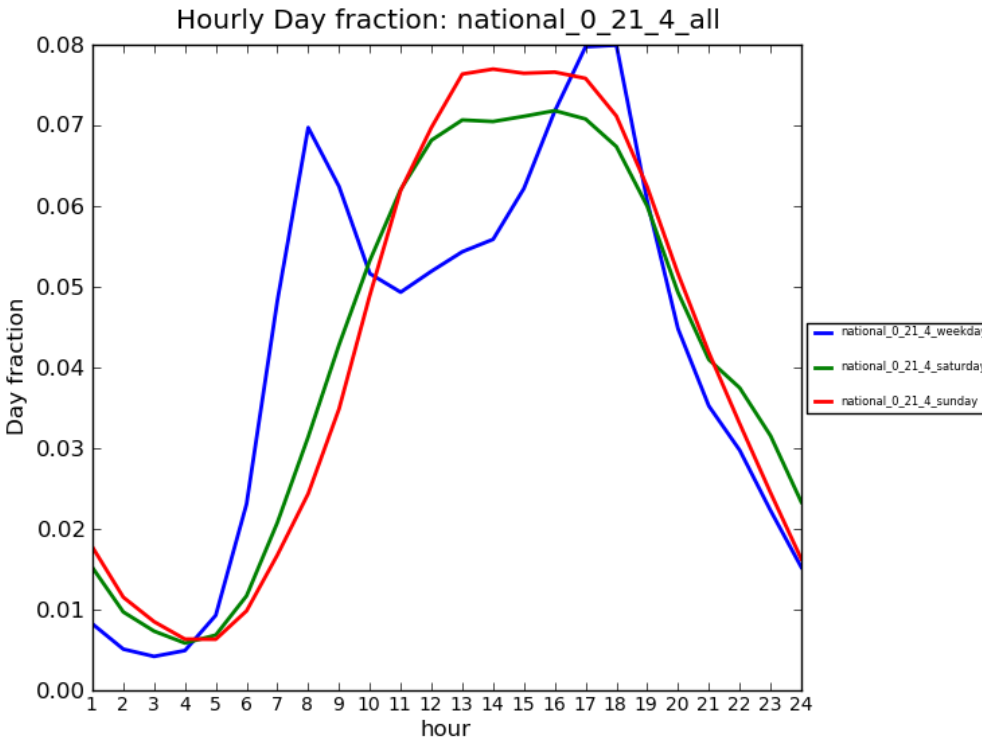
- SMOKE-MOVES now uses MOVES2014 and new SCCs that map more cleanly to MOVES
- Use county-specific age distributions
- Speciation done in MOVES (upgrades for CB05+CB6)
- Revised long-haul extended idle
- Revised long-haul splits: now region specific splits
- Incorporated monitoring data into temporalization
- More detailed spatial surrogates (e.g., truck stops)
- More representative counties (284 vs 163)
- Improved performance -> about the same time required

Improved Onroad Temporal Profiles

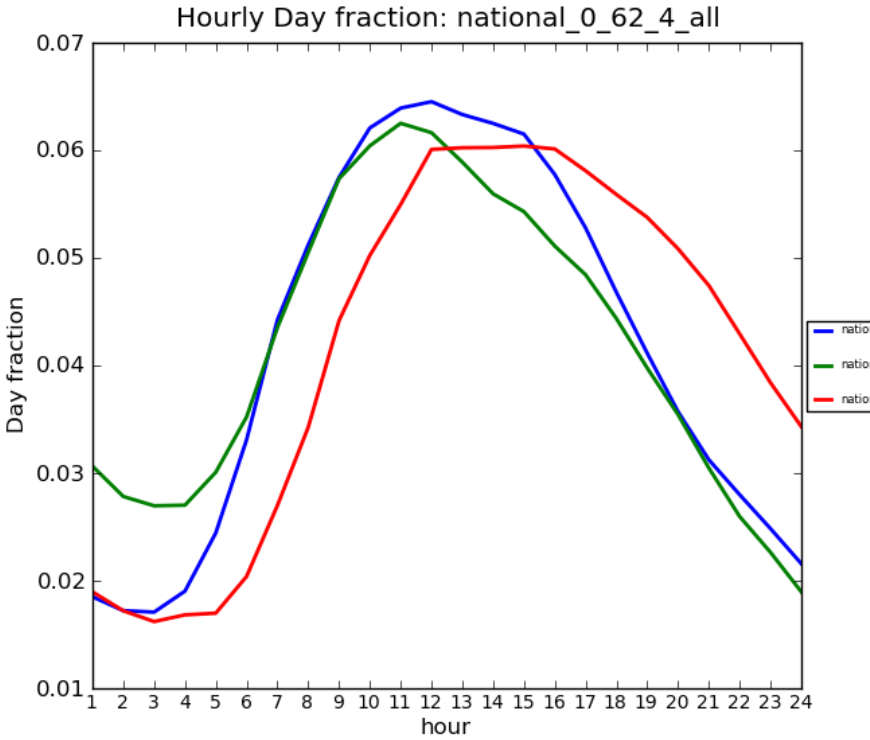
- Improved temporal profiles with 2012 Vehicle Travel Information System (VTRIS) data
  - Reported traffic count data to the Federal Highway Administration (FHWA)
  - Varies by state, HPMS vehicle (10, 20, 30, …) and road type
  - Distinct hourly / diurnal profiles for weekdays/Sat/Sunday
  - Day of the week profiles (i.e. Monday vs Tuesday vs …)
- Combined with more refined use of state submitted temporal information via NEIv2

National Diurnal Temporal Profiles

- Days of week: Blue weekday, Green Sat, Red Sun



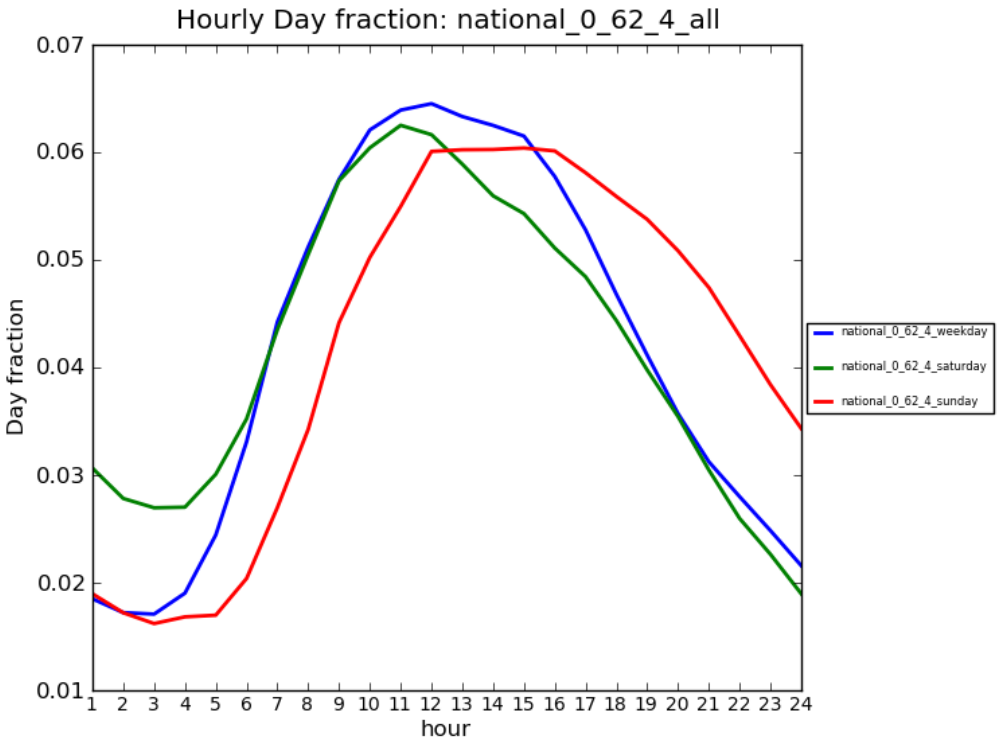
Passenger cars
Urban restricted



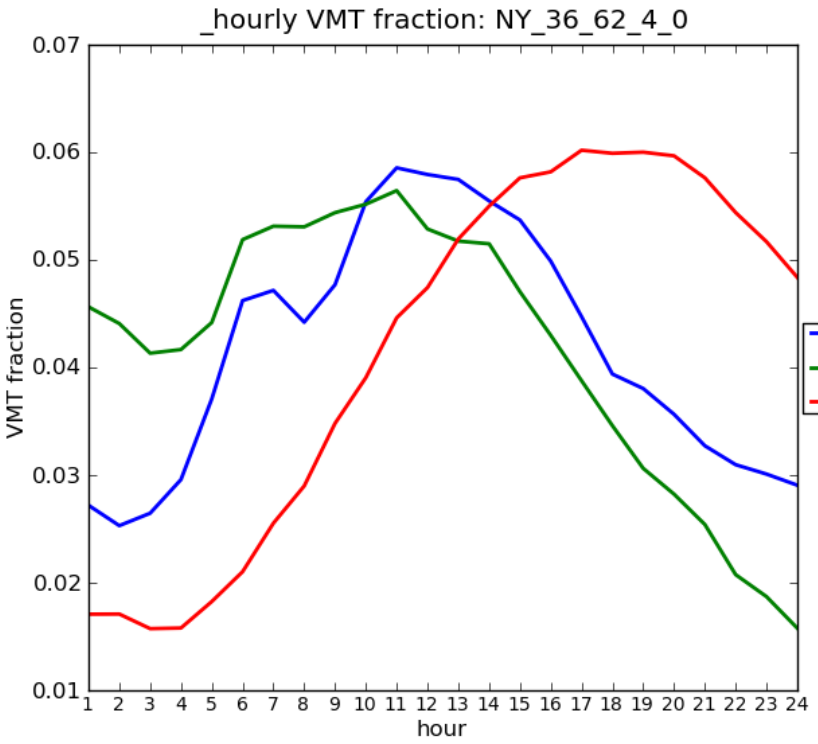
Combination truck long-haul
Urban restricted

State Diurnal Temporal Profiles

- Days of week: Blue weekday, Green Sat, Red Sun



National

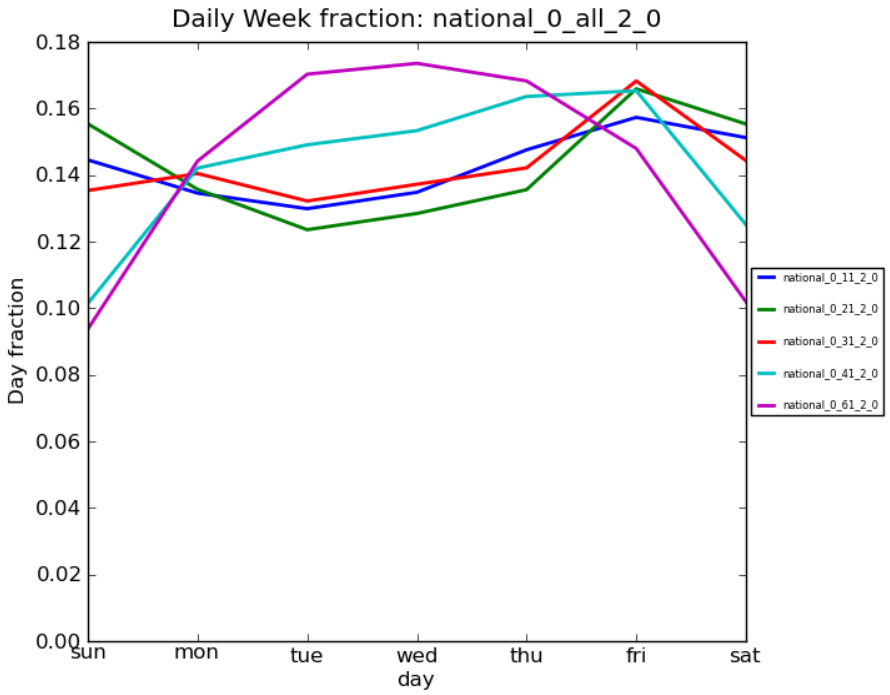


NY

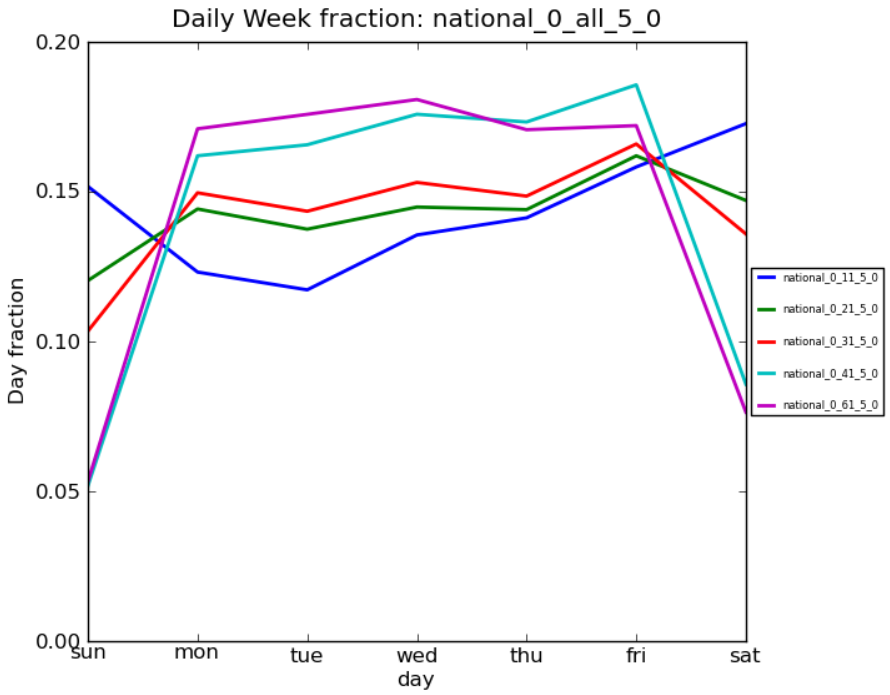
Combination truck long-haul
Urban restricted

National Day of Week Temporal Profiles

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



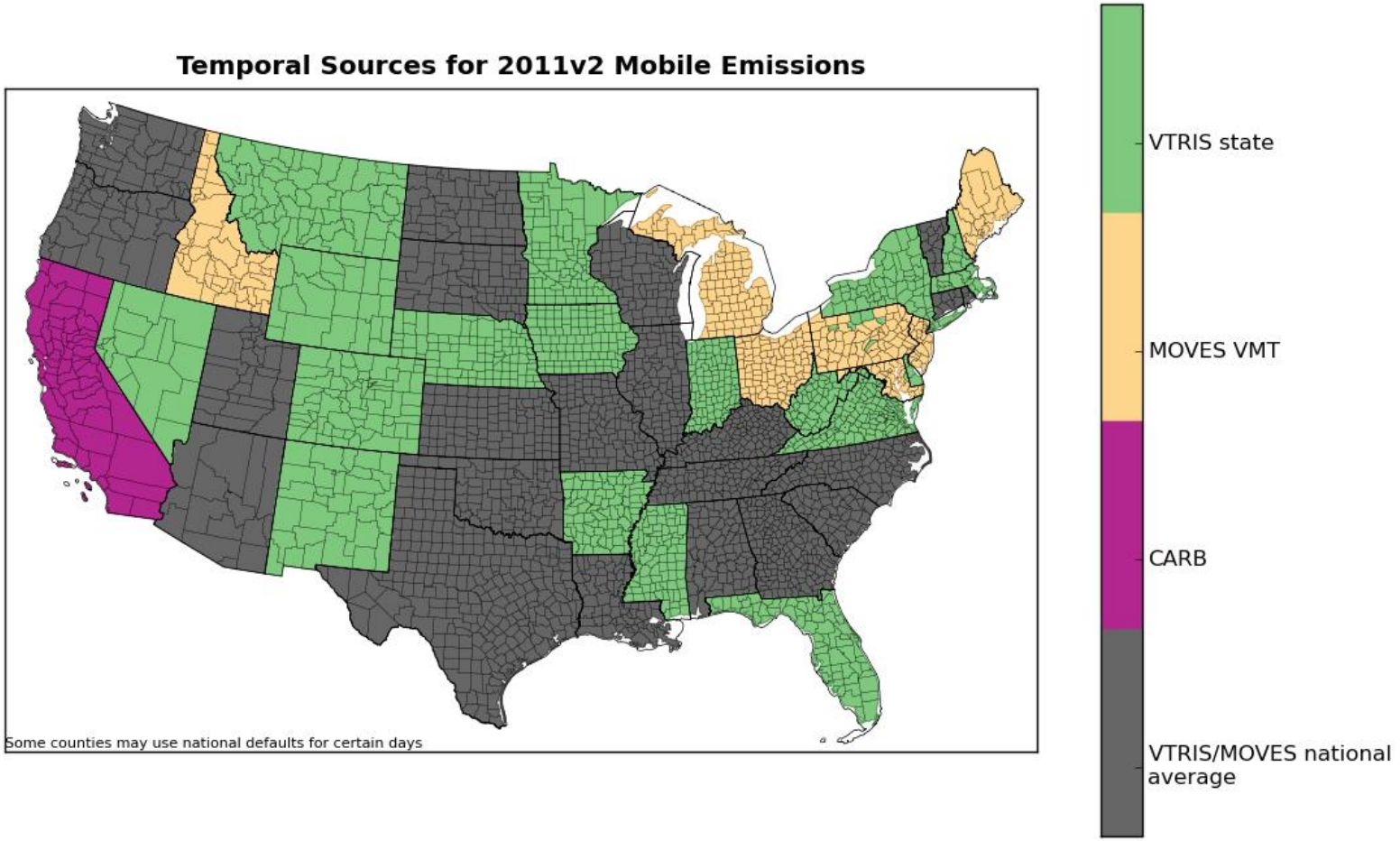
Rural restricted:
light-duty have Friday peak



Urban unrestricted:
more traffic weekdays

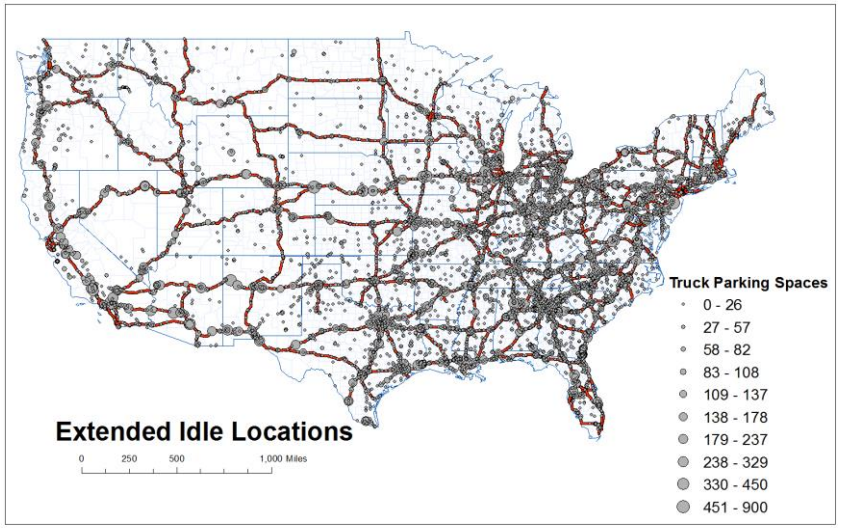
Geographic specific temporal profiles

- Many states and some counties have location specific profiles



Improved Onroad Hotelling

- Improved hotelling in SMOKE-MOVES
  - Covers overnight idling
  - Extended idle and APU
- States were able to submit hotelling hours by county
- For EPA estimates, used combination long-haul trucks VMT on restricted roads (urban + rural) to distribute hotelling hours
- Created temporal profile
- Updated spatial surrogate



Questions?

- Any questions on onroad emissions processing?

Final Merging and QA

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

Sector Merge Script and Sector List

sector	sectorcase	sectbaseyr	mrgapproach	Prevyr spinup	endzip	speciation	Merge sector
afdust	2011eh_cb05_v6_11g	2011	week_Y	SectBaseYr	N	cmaq_cb05_soa	N
afdust_adj	2011eh_cb05_v6_11g	2011	all	SectBaseYr	Y	cmaq_cb05_soa	Y
ag	2011eh_cb05_v6_11g	2011	all	SectBaseYr	Y	cmaq_cb05_soa	Y
agfire	2011eh_cb6v2_v6_11g	2011	week_Y	SectBaseYr	N		Y
beis	2011eh_cb6v2_v6_11g	2011	all	actualMet	N		Y
c1c2rail	2011eh_cb6v2_v6_11g	2011	mwdss_N	SectBaseYr	N		Y
c3marine	2011eh_cb6v2_v6_11g	2011	aveday_N	SectBaseYr	N		Y
nonpt	2011eh_cb6v2_v6_11g	2011	week_Y	SectBaseYr	N		Y
nonroad	2011eh_cb6v2_v6_11g	2011	mwdss_Y	SectBaseYr	N		Y
np_oilgas	2011eh_cb6v2_v6_11g	2011	week_Y	SectBaseYr	N		Y
ocean_cl2	none	2011	$OCL2ROOT$ GRID$EXT	SectBaseYr	N		Y
onroad	2011eh_cb6v2_v6_11g	2011	all	SectBaseYr	Y		Y
onroad_ca_adj	2011eh_cb6v2_v6_11g	2011	all	SectBaseYr	Y		Y
pt_oilgas	2011eh_cb6v2_v6_11g	2011	mwdss_Y	SectBaseYr	N		Y
ptegu	2011eh_cb6v2_v6_11g	2011	all	SectBaseYr	Y		Y
ptfire	2011eh_cb6v2_v6_11g	2011	all	SectBaseYr	Y		N
ptnonipm	2011eh_cb6v2_v6_11g	2011	mwdss_Y	SectBaseYr	N		Y
ptprescfire3D	2011eh_cb6v2_v6_11g	2011	all	SectBaseYr	N		N
ptwildfire3D	2011eh_cb6v2_v6_11g	2011	all	SectBaseYr	N		N
rwc	2011eh_cb6v2_v6_11g	2011	all	SectBaseYr	Y		Y
othpt	2011eh_cb6v2_v6_11g	2011	mwdss_N	SectBaseYr	N		N

QA of Merged Emissions

- Look at the mrggrid logs to ensure that the correct case/sector files are merging.
- Generate domain totals of the 2D and inline files and compare back to the sum of the sector SMOKE annual reports.
- Check the size of the 2D merged emissions files to make sure that the file size is the same for each day (corrupted files will be smaller)

SMOKE 3.6 Updates

- MOVES 2014 support
  - Speciation done within MOVES
  - Computational speed-ups support handling more reference counties in the same time as before
  - New rate-per-hour mode for extended idling of trucks
  - Control factors can be input to Movesmrg by representative county and pollutant
- Better support for source apportionment
- Includes BEIS 3.6.1
- New temporal profile and cross reference format
  - Database-friendly .csv format with more flexibility

Questions?

- Any final questions on first half of training?