Technical Support Document (TSD)
Preparation of Emissions Inventories for the Version 7.1
2015 Emissions Modeling Platform

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TABLE OF CONTENTS

List of Tables

List of Figures

List of Appendices

Acronyms

AE5	CMAQ Aerosol Module, version 5, introduced in CMAQ v4.7
AE6	CMAQ Aerosol Module, version 6, introduced in CMAQ v5.0
AEO	Annual Energy Outlook
AERMOD	American Meteorological Society/Environmental Protection Agency Regulatory Model
NBAFM	Naphthalene, Benzene, Acetaldehyde, Formaldehyde and Methanol
BEIS	Biogenic Emissions Inventory System
BELD	Biogenic Emissions Land use Database
Bgal	Billion gallons
BPS	Bulk Plant Storage
BTP	Bulk Terminal (Plant) to Pump
C1/C2	Category 1 and 2 commercial marine vessels
C3	Category 3 (commercial marine vessels)
CAEP	Committee on Aviation Environmental Protection
CAIR	Clean Air Interstate Rule
CAMD	EPA's Clean Air Markets Division
CAMx	Comprehensive Air Quality Model with Extensions
CAP	Criteria Air Pollutant
CARB	California Air Resources Board
CB05	Carbon Bond 2005 chemical mechanism
CBM	Coal-bed methane
CEC	North American Commission for Environmental Cooperation
CEMS	Continuous Emissions Monitoring System
CEPAM	California Emissions Projection Analysis Model
CISWI	Commercial and Industrial Solid Waste Incinerators
Cl	Chlorine
CMAQ	Community Multiscale Air Quality
CMV	Commercial Marine Vessel
CO	Carbon monoxide
CSAPR	Cross-State Air Pollution Rule
E0, E10, E85	0%, 10% and 85% Ethanol blend gasoline, respectively
EBAFM	Ethanol, Benzene, Acetaldehyde, Formaldehyde and Methanol
ECA	Emissions Control Area
EEZ	Exclusive Economic Zone
EF	Emission Factor
EGU	Electric Generating Units
EIS	Emissions Inventory System
EISA	Energy Independence and Security Act of 2007
EPA	Environmental Protection Agency
EMFAC	Emission Factor (California's onroad mobile model)
FAA	Federal Aviation Administration
FAPRI	Food and Agriculture Policy and Research Institute
FASOM	Forest and Agricultural Section Optimization Model
FCCS	Fuel Characteristic Classification System
FF10	Flat File 2010
FIPS	Federal Information Processing Standards
FHWA	Federal Highway Administration
HAP	Hazardous Air Pollutant

HCl	Hydrochloric acid
HDGHG	Heavy-Duty Vehicle Greenhouse Gas
Hg	Mercury
HMS	Hazard Mapping System
HPMS	Highway Performance Monitoring System
HWC	Hazardous Waste Combustion
HWI	Hazardous Waste Incineration
ICAO	International Civil Aviation Organization
ICI	Industrial/Commercial/Institutional (boilers and process heaters)
ICR	Information Collection Request
IDA	Inventory Data Analyzer
I/M	Inspection and Maintenance
IMO	International Marine Organization
IPAMS	Independent Petroleum Association of Mountain States
IPM	Integrated Planning Model
ITN	Itinerant
LADCO	Lake Michigan Air Directors Consortium
LDGHG	Light-Duty Vehicle Greenhouse Gas
LPG	Liquefied Petroleum Gas
MACT	Maximum Achievable Control Technology
MARAMA	Mid-Atlantic Regional Air Management Association
MATS	Mercury and Air Toxics Standards
MCIP	Meteorology-Chemistry Interface Processor
Mgal	Million gallons
MMS	Minerals Management Service (now known as the Bureau of Energy Management, Regulation and Enforcement (BOEMRE)
MOVES	Motor Vehicle Emissions Simulator
MSA	Metropolitan Statistical Area
MSAT2	Mobile Source Air Toxics Rule
MTBE	Methyl tert-butyl ether
MWRPO	Mid-west Regional Planning Organization
NCD	National County Database
NEEDS	National Electric Energy Database System
NEI	National Emission Inventory
NESCAUM	Northeast States for Coordinated Air Use Management
NESHAP	National Emission Standards for Hazardous Air Pollutants
NH_3	Ammonia
NIF	NEI Input Format
NLCD	National Land Cover Database
NLEV	National Low Emission Vehicle program
nm	nautical mile
NMIM	National Mobile Inventory Model
NOAA	National Oceanic and Atmospheric Administration
NODA	Notice of Data Availability
NONROAD	OTAQ's model for estimation of nonroad mobile emissions
NO_X	Nitrogen oxides
NSPS	New Source Performance Standards
NSR	New Source Review
OAQPS	EPA's Office of Air Quality Planning and Standards
OHH	Outdoor Hydronic Heater

OTAQ	EPA's Office of Transportation and Air Quality
ORIS	Office of Regulatory Information System
ORD	EPA's Office of Research and Development
ORL	One Record per Line
OTC	Ozone Transport Commission
PADD	Petroleum Administration for Defense Districts
PF	Projection Factor, can account for growth and/or controls
PFC	Portable Fuel Container
$PM_{2.5}$	Particulate matter less than or equal to 2.5 microns
PM_{10}	Particulate matter less than or equal to 10 microns
ppb, ppm	Parts per billion, parts per million
RBT	Refinery to Bulk Terminal
RFS2	Renewable Fuel Standard
RIA	Regulatory Impact Analysis
RICE	Reciprocating Internal Combustion Engine
RWC	Residential Wood Combustion
RPO	Regional Planning Organization
RVP	Reid Vapor Pressure
SCC	Source Classification Code
SEMAP	Southeastern Modeling, Analysis, and Planning
SESARM	Southeastern States Air Resource Managers
SESQ	Sesquiterpenes
SMARTFIRE	Satellite Mapping Automated Reanalysis Tool for Fire Incident Reconciliation
SMOKE	Sparse Matrix Operator Kernel Emissions
SO_2	Sulfur dioxide
SOA	Secondary Organic Aerosol
SI	Spark-ignition
SIP	State Implementation Plan
SPDPRO	Hourly Speed Profiles for weekday versus weekend
SPPD	Sector Policies and Programs Division
TAF	Terminal Area Forecast
TCEQ	Texas Commission on Environmental Quality
TOG	Total Organic Gas
TSD	Technical support document
ULSD	Ultra Low Sulfur Diesel
USDA	United States Department of Agriculture
VOC	Volatile organic compounds
VMT	Vehicle miles traveled
VPOP	Vehicle Population
WRAP	Western Regional Air Partnership
WRF	Weather Research and Forecasting Model

1 Introduction

The U.S. Environmental Protection Agency (EPA) developed an air quality modeling platform for air toxics and criteria air pollutants that represents the year 2015 based on the 2014 National Emissions Inventory (NEI), version 2 (2014NEIv2). The air quality modeling platform consists of all the emissions inventories and ancillary data files used for emissions modeling, as well as the meteorological, initial condition, and boundary condition files needed to run the air quality model. This document focuses on the emissions modeling component of the 2015 modeling platform, which includes the emission inventories, the ancillary data files, and the approaches used to transform inventories for use in air quality modeling. Many emissions inventory components of this air quality modeling platform are based on the 2014NEIv2, including projections to year 2015 for some emissions sectors.

This 2015 modeling platform includes all criteria air pollutants and precursors (CAPs), and a group of hazardous air pollutants (HAPs) and diesel particulate matter. The group of HAPs are those explicitly used by the chemical mechanism in the Community Multiscale Air Quality (CMAQ) model for ozone/particulate matter (PM): chlorine (Cl), hydrogen chloride (HCl), benzene, acetaldehyde, formaldehyde, methanol, naphthalene. The platform was used to support air quality modeling applications using CMAQ version 5.2. The modeling domain includes the lower 48 states and parts of Canada and Mexico.

The CMAQ model requires hourly and gridded emissions of chemical species that correspond to CAPs and specific HAPs. The chemical mechanism used by CMAQ for this platform is called Carbon Bond version 6-CMAQ (CB6-CMAQ) and includes important reactions for simulating ozone formation, nitrogen oxides (NOx) cycling, and formation of secondary aerosol species. It is basically the same as the CB6 used in the 2011v6.3 platform described in (Hildebrandt Ruiz and Yarwood, 2013) except that CB6-CMAQ removes naphthalene from the lumped species group “XYL” and treats it explicitly. In addition, many additional HAPs are included to support the NATA analysis. The CAMx model uses a similar, but slightly different, chemical mechanism, as described in Section **Error! Reference source not found.**.

The 2015 platform consists of one ‘complete’ emissions case: the 2015 base case, i.e., 2015fd_cb6_15j. This platform accounts for atmospheric chemistry and transport within a state of the art photochemical grid model. In the case abbreviation 2015fd_cb6_15j, 2015 is the year represented by the emissions; the “f” represents the base year platform iteration, which in this case is 2014 (the previous platform, which was a 2011-based platform, was “e”); the “d” stands for the fourth set of emissions modeled for a 2014-based modeling platform.

The emissions data in the 2015 platform are primarily based on the 2014NEIv2 for point sources, nonpoint sources, commercial marine vessels (CMV), onroad and nonroad mobile sources, and fires. Some platform categories are based on more disaggregated data than are made available in the NEI. For example, in the platform, onroad mobile source emissions are representated as hourly emissions by vehicle type, fuel type process and road type. In contrast, the onroad emissions in the 2014NEI are developed using the same inputs, but those emissions are aggregated to vehicle type/fuel type totals and annual temporal resolution. In addition, emissions from Canada and Mexico are used for the platform but are not part of the NEI. Temporal, spatial and other changes in emissions between the 2014NEI and the emissions input into the platform are described in Section 2 of this TSD. Point source emissions include some updates for the year 2015.

The primary emissions modeling tool used to create the air quality model-ready emissions was the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system (http://cmascenter.org/smoke), version 4.5

(SMOKE 4.5) with some updates. Emissions files were created for a 36-km national grid, 36US3, and two 12-km national grids, "12US1" and "12US2", all of which include all of the contiguous states and parts of Canada and Mexico as shown in Figure 3-1.

The gridded meteorological model used to provide input data for the emissions modeling was developed using the Weather Research and Forecasting Model (WRF, http://wrf-model.org) version 3.8, Advanced Research WRF core (Skamarock, et al., 2008). The WRF Model is a mesoscale numerical weather prediction system developed for both operational forecasting and atmospheric research applications. The WRF was run for 2015 over a domain covering the continental U.S. at a 12km resolution with 35 vertical layers. The run for this platform included high resolution sea surface temperature data from the Group for High Resolution Sea Surface Temperature (GHRSST) (see https://www.ghrsst.org/) and is given the EPA meteorological case label "15j." The full case name includes this abbreviation following the emissions portion of the case name to fully specify the name of the case as "2015fd_15j."

This document contains five sections and several appendices. Section 2 describes the 2015 inventories input to SMOKE. Section 3 describes the emissions modeling and the ancillary files used with the emission inventories. Section 4 provides references. The Appendices provide additional details about specific technical methods or data.

2 2015 Emission Inventories and Approaches

This section describes the emissions data that make up the 2015 platform. The starting point for the stationary source emission inputs is the 2014NEIv2 or more detailed temporal/spatial resolution data used to build the NEI, with some sectors projected to 2015, and other adjustments made to support modeling as described here. Documentation for the 2014NEIv2, including a TSD, is available from https://www.epa.gov/air-emissions-inventories/2014-national-emissions-inventory-nei-technical-support-document-tsd.

The NEI data for CAPs are largely compiled from data submitted by state, local and tribal (S/L/T) air agencies. HAP emissions data are also from the S/L/T agencies, but, are often augmented by the EPA because they are voluntarily submitted. The EPA uses the Emissions Inventory System (EIS) to compile the NEI. The EIS includes hundreds of automated quality assurance (QA) checks to help improve data quality, and also supports tracking release point (e.g., stack) coordinates separately from facility coordinates. The EPA collaborated extensively with S/L/T agencies to ensure a high quality of data in the 2014NEI. A targeted review of the data was conducted between the 2014NEIv1 and 2014NEIv2 using initial risk projections to identify potential outliers as a part of the NATA review process.

Point source data for the year 2015 as submitted to EIS were used for this study. EPA used the SMARTFIRE2 system to develop 2015 fire emissions. SMARTFIRE2 categorizes all fires as either prescribed burning or wildfire categories and includes improved emission factor estimates for prescribed burning. Onroad mobile source emissions for year 2015 were developed using MOVES2014a. Nonroad mobile source emissions were developed by running MOVES2014a for 2015. Canadian emissions reflect year 2013 and Mexican emissions were interpolated to year 2015.

Onroad and nonroad mobile source emissions were developed using the Motor Vehicle Emission Simulator (MOVES). MOVES2014a was used with S/L inputs, where provided, in combination with EPA-generated default data. The 2014 NEI is the first use of MOVES for nonroad emissions. MOVES2014a replaces the National Mobile Inventory Model (NMIM) as the interface for using the NONROAD2008 model, ensuring that the gasoline fuels used for nonroad equipment are consistent with those used for onroad vehicles and using newer data to estimate the HAPs than had been used in NMIM.

Onroad emissions for the 2015 platform were developed based on emissions factors output from MOVES2014a for the year 2015 run with inputs derived from the 2014NEIv2.

The 2014 NEI includes five data categories: point sources, nonpoint (formerly called "stationary area") sources, nonroad mobile sources, onroad mobile sources, and events consisting of fires. The NEI uses 60 sectors to further describe the emissions, with an additional biogenic sector generated from a summation of the gridded, hourly biogenic data used in the emissions modeling platform. In addition to the NEI data, emissions from the Canadian and Mexican inventories and several other non-NEI data sources are included in the 2015 platform.

The methods used to process emissions for this study are similar to those documented for EPA's Version 7.1, 2014 Emissions Modeling Platform that was also used for version 2 of the 2014 National Air Toxics Assessment (NATA), with some exceptions. One exception is that many fewer HAPs are included in this platform. Also, many emissions inventories and inputs were updated to the year 2015 for this study. A technical support document (TSD) for the 2014v7.1 platform is available here https://www.epa.gov/air-emissions-modeling/2014-version-71-technical-support-document-tsd (EPA, 2018b) and includes additional details regarding the data preparation and emissions modeling, with the exception of the HAP speciation and any updates specific to 2015.

Compared to the 2014v7.1 emissions modeling platform, which is based directly on the 2014NEIv2, the 2015v7.1 emissions modeling platform includes emissions for the year 2015 for some data categories. The point source emission inventories for platform include partially updated emissions for 2015. Agricultural and wildland fire emissions represent the year 2015. Most area source sectors use 2014NEIv2 emissions estimates except for commercial marine vehicles (CMV), fertilizer emissions, oil and gas emissions, and onroad and nonroad mobile source emissions. For CMV, SO_2 emissions were updated to reflect new rules on sulfur emissions that took effect in the year 2015. For fertilizer ammonia emissions, a 2015-specific emissions inventory is used in this platform. Area source oil and gas emissions were projected from 2014NEIv2 to better represent 2015. Onroad and nonroad emissions for the year 2015 were developed based on MOVES2014a outputs for 2015, and the activity data used to compute the onroad emissions were projected from 2014 to 2015.

The emissions modeling process performed using SMOKE v4.5, apportions the emissions inventories into the grid cells used by CMAQ and temporalizes the emissions into hourly values. In addition, the pollutants in the inventories (e.g., NOx, PM and VOC) are split into the chemical species needed by CMAQ. For the purposes of preparing the air quality model-ready emissions, the NEI was split into finer-grained sectors used for emissions modeling; and emissions from sources other than the NEI are added, such as the Canadian, Mexican, and offshore inventories. The significance of an emissions modeling or "platform sector" is that the data are run through the SMOKE programs independently from the other sectors except for the final merge (Mrggrid). The final merge program combines the sector-specific gridded, speciated, hourly emissions together to create CMAQ-ready emission inputs. For biogenic emissions, the CMAQ model allows for biogenic emissions to be included in the CMAQ-ready emissions inputs, or for biogenic emissions to be computed within CMAQ itself (the "inline" option). This study uses the inline biogenics option.

Table 2-1 presents the sectors in the 2015 platform used to develop the year 2015 emissions for this project. and how they generally relate to the 2014NEIv2 as a starting point. The platform sector abbreviations are provided in italics. These abbreviations are used in the SMOKE modeling scripts, inventory file names, and throughout the remainder of this document. Annual 2015 emission summaries for the U.S. anthropogenic sectors are shown in Table 2-2 (i.e., biogenic emissions are excluded). Table

2-3 provides a summary of emissions for the anthropogenic sectors containing Canadian, Mexican and offshore sources.

Table 2-1. Platform sectors for the 2015 emissions modeling platform

Platform Sector *(Abbrev)*	NEI Category	Description and resolution of the data input to SMOKE
EGUs (*ptegu)*	Point	2015 point source EGUs. Replaced with hourly 2015 Continuous Emissions Monitoring System (CEMS) values for NOX and SO2, where the units are matched to the NEI. Emissions for all sources not matched to CEMS data come from 2015 NEI point inventory. Annual resolution for sources not matched to CEMS data, hourly for CEMS sources.
Point source oil and gas (*pt_oilgas)*	Point	2015 NEI point sources that include oil and gas production emissions processes based on facilities with the following NAICS: 211* (Oil and Gas Extraction), 2212* (Natural Gas Distribution), 213111 (Drilling Oil and Gas Wells), 213112 (Support Activities for Oil and Gas Operations), 4861* (Pipeline Transportation of Crude Oil), 4862* (Pipeline Transportation of Natural Gas). Includes U.S. offshore oil production. The portion of the 2015 NEI point inventory oil and gas inventory that was carried forward from 2014NEIv2 (i.e. not updated to 2015 in EIS) was projected to year 2015 estimates. Annual resolution.
Remaining non-EGU point (*ptnonipm*)	Point	All 2015 NEI point source records not matched to the ptegu or pt_oilgas sectors. Includes all aircraft and airport ground support emissions and some rail yard emissions. Annual resolution.
Point source fire (*ptfire*)	Fires	Point source day-specific wildfires and prescribed fires for 2015 computed using SMARTFIRE 2. Fires over 20,000 acres on a single day allocated to overlapping grid cells.
Point Source agricultural fires (*ptagfire*)	Nonpoint	Agricultural fire sources that were developed by EPA as point and day-specific emissions; they were put into the nonpoint data category of the NEI, but in the platform, they are treated as point sources.
Agricultural (*ag*)	Nonpoint	2014NEIv2 nonpoint livestock and fertilizer application emissions. Livestock includes ammonia and other pollutants (except PM2.5). Fertilizer includes only ammonia. County and annual resolution.
Area fugitive dust (*afdust_adj*)	Nonpoint	PM_{10} and $PM_{2.5}$ fugitive dust sources from the 2014NEIv2 nonpoint inventory; including building construction, road construction, agricultural dust, and road dust. The emissions modeling adjustment applies a transport fraction and a zero-out based on 2015 meteorology (precipitation and snow/ice cover). County and annual resolution.
Biogenic (*beis*)	Nonpoint	Biogenic emissions were left out of the CMAQ-ready merged emissions, in favor of inline biogenics produced during the CMAQ model run itself.
C1 and C2 commercial marine (*cmv_c1c2*)	Nonpoint	2014NEIv2 Category 1 (C1) and Category 2 (C2), commercial marine vessel (CMV) emissions. County and annual resolution.

Platform Sector *(Abbrev)*	NEI Category	Description and resolution of the data input to SMOKE
C3 commercial marine (*cmv_c3*)	Nonpoint	Within state and federal waters, 2014NEIv2 Category 3 commercial marine vessel (CMV) emissions. Outside of state and federal waters, emissions are based on the Emissions Control Area (ECA) inventory. Point (to allow for plume rise) and annual resolution.
Remaining nonpoint (*nonpt*)	Nonpoint	2014NEIv2 nonpoint sources not included in other platform sectors. County and annual resolution.
Nonpoint source oil and gas (*np_oilgas)*	Nonpoint	2014NEIv2 nonpoint sources from oil and gas-related processes, projected to year 2015 estimates. County and annual resolution.
Locomotive (*rail*)	Nonpoint	Rail locomotives emissions from the 2014NEIv2. County and annual resolution.
Residential Wood Combustion (*rwc*)	Nonpoint	2014NEIv2 nonpoint sources with residential wood combustion (RWC) processes. County and annual resolution.
Nonroad (*nonroad*)	Nonroad	2015 nonroad equipment emissions developed with the MOVES2014a. MOVES was run for 2014 and 2016, and the resulting emissions were interpolated to 2015. MOVES was used for all states except California, which submitted their own emissions for the 2014NEIv2 and for the year 2017, from which 2015 estimates were interpolated. County and monthly resolution.
Onroad (*onroad*)	Onroad	2015 onroad mobile source gasoline and diesel vehicles from parking lots and moving vehicles. Includes the following modes: exhaust, extended idle, auxiliary power units, evaporative, permeation, refueling, and brake and tire wear. For all states except California, developed using winter and summer MOVES emission factors tables produced by MOVES2014a.
Onroad California (*onroad_ca_adj*)	Onroad	California-provided CAP and metal HAP onroad mobile source gasoline and diesel vehicles from parking lots and moving vehicles based on Emission Factor (EMFAC), gridded and temporalized using MOVES2014a. Volatile organic compound (VOC) HAP emissions derived from California-provided VOC emissions and MOVES-based speciation. California estimates for 2014 and 2017 were interpolated to 2015 values.
Onroad Canada (*onroad_can*)	Non-US	Monthly year 2013 Canada (province resolution) onroad mobile inventory.
Onroad Mexico (*onroad_mex*)	Non-US	Monthly year Mexico (municipio resolution) onroad mobile inventory, with 2015 emissions values interpolated from 2014 and 2018 inventories.
Other area fugitive dust sources (*othafdust_adj*)	Non-US	Area fugitive dust sources from Canada 2013 inventory with transport fraction and snow/ice adjustments based on 2015 meteorological data. Annual and province resolution.

Platform Sector *(Abbrev)*	NEI Category	Description and resolution of the data input to SMOKE
Other nonpoint and nonroad (*othar*)	Non-US	Year 2013 Canada (province resolution) and projected year 2015 Mexico (municipio resolution, interpolated from 2014 and 2018 values) nonpoint and nonroad mobile inventories, annual resolution.
Other point sources not from the NEI (*othpt*)	Non-US	Point sources from Canada's 2013 inventory, and Mexico point source emissions for 2015 (interpolated from 2014 and 2018). Annual resolution.
Point fires in Mexico and Canada (*ptfire_othna*)	Non-US	Point source day-specific wildfires and prescribed fires for 2015 are computed from SMARTFIRE 2 in Canada and Mexico. Caribbean, Central American, and other international fires are from 2015 v1.5 of the Fire INventory (FINN) from National Center for Atmospheric Research (NCAR) fires (NCAR, 2016 and Wiedinmyer, C., 2011).

Table 2-2. 2015 Continental United States Emissions by Sector (tons/yr in 48 states + D.C.)

Sector	CO	NH_3	NO_x	PM_{10}	$PM_{2.5}$	SO_2	VOC
afdust_adj				6,093,367	857,261		
ag		2,823,395					179,970
cmv_c1c2	47,183	120	260,338	6,493	6,168	3,453	4,840
cmv_c3	10,885	25	108,268	4,248	3,832	38,826	5,043
nonpt	2,680,775	121,229	758,152	608,827	496,454	162,231	3,672,687
np_oilgas	686,168	15	719,934	17,746	17,480	38,963	3,206,411
nonroad	12,405,416	2,211	1,375,025	139,410	132,017	3,129	1,622,303
onroad	23,064,322	104,472	4,401,420	285,167	144,312	27,173	2,199,205
ptagfire	382,760	53,353	11,971	62,034	43,724	3,719	23,711
ptfire	21,180,425	347,360	275,352	2,142,471	1,815,654	154,996	4,993,305
ptegu	625,780	19,811	1,451,134	176,516	136,106	2,293,080	33,581
ptnonipm	1,967,804	73,358	1,108,414	418,371	273,483	788,604	834,143
pt_oilgas	190,337	1,244	390,734	12,372	11,856	43,422	142,197
rail	118,367	363	672,558	20,728	19,154	700	34,739
rwc	2,098,907	15,331	30,493	314,466	313,945	7,684	338,465
Continental U.S.	**65,459,130**	**3,562,287**	**11,563,793**	**10,302,215**	**4,271,445**	**3,565,979**	**17,290,600**

Table 2-3. 2015 Continental United States 12US1 Emissions by Sector (tons/yr in 48 states + D.C.)

Sector	CO	NH_3	NO_X	PM_{10}	$PM_{2.5}$	SO_2	VOC
Canada othafdust				2,232,563	438,196		
Canada othar	2,892,737	497,580	652,907	425,822	237,155	70,080	1,128,917
Canada onroad_can	2,130,822	8,514	478,221	28,406	21,623	1,614	193,264
Canada othpt	1,102,931	17,323	646,978	91,095	47,322	999,876	782,445
Canada ptfire_othna	10,277,333	290,735	339,883	1,216,218	1,109,341	85,204	2,853,915
Canada Subtotal	**16,403,822**	**814,152**	**2,117,989**	**3,994,105**	**1,853,636**	**1,156,775**	**4,958,542**
Mexico othar	236,143	203,945	216,175	114,754	53,727	7,661	512,070
Mexico onroad_mex	1,825,267	2,724	437,330	14,935	10,744	6,047	158,562
Mexico othpt	196,410	4,851	456,220	72,957	57,378	509,144	68,615
Mexico ptfire_othna	81,991	1,390	7,168	10,654	8,557	641	28,294
Mexico Subtotal	**2,339,811**	**212,911**	**1,116,894**	**213,300**	**130,406**	**523,494**	**767,541**
Offshore cmv_c1c2	56,393	184	283,431	9,193	8,918	2,236	5,248
Offshore cmv_c3	77,449	68	854,639	47,205	43,618	358,452	34,059
Offshore pt_oilgas	50,046	15	48,688	668	666	502	48,167
2015 Total non-U.S.	**18,850,073**	**1,027,262**	**3,567,003**	**4,217,266**	**1,993,627**	**1,683,006**	**5,779,497**

The emission inventories in SMOKE input formats for the 2015 platform are available from the EPA's Air Emissions Modeling website for the platform: https://www.epa.gov/air-emissions-modeling/2014-2016-version-7-air-emissions-modeling-platforms, under the section entitled "2015v7.1 (alpha) Platform" The platform "README" file indicates the particular zipped files associated with each platform sector.

The remainder of Section 2 provides details about the data contained in each of the platform sectors. Different levels of detail are provided for different sectors depending on the availability of reference information for the data, the degree of changes or manipulation of the data needed to prepare it for input to SMOKE, and whether the 2015 platform emissions are significantly different from the 2014NEIv2.

2.1 Point sources (ptegu, pt_oilgas and ptnonipm)

Point sources are sources of emissions for which specific geographic coordinates (e.g., latitude/longitude) are specified, as in the case of an individual facility. A facility may have multiple emission release points that may be characterized as units such as boilers, reactors, spray booths, kilns, etc. A unit may have multiple processes (e.g., a boiler that sometimes burns residual oil and sometimes burns natural gas). With a couple of minor exceptions, this section describes only NEI point sources within the contiguous U.S. The offshore oil platform (pt_oilgas sector) and category 3 CMV emissions (cmv_c3 sector) are processed by SMOKE as point source inventories and are discussed later in this section. This section describes NEI point sources within the contiguous U.S. and the offshore oil platforms which are processed by SMOKE as point source inventories, as described in Section 2.5.1. A comprehensive description of how EGU emissions were characterized and estimated in the 2014 NEI is located in Section 3.4 in the 2014NEIv2 TSD (EPA, 2018a).

A complete NEI is developed every three years, with 2014 being the most recently finished complete NEI. A comprehensive description about the development of the 2014NEIv2 is available in the 2014NEIv2 TSD (EPA, 2018a). Point inventories are also available in EIS for intermediate years such as 2015. In this intermediate point inventory, larger sources are updated with emissions for year 2015, while other sources are either carried forward from 2014NEIv2 or are closed.

In preparation for modeling, the complete set of point sources in the NEI was exported from EIS for the year 2015 into the Flat File 2010 (FF10) format that is compatible with SMOKE (see https://www.cmascenter.org/smoke/documentation/4.5/html/ch08s02s08.html) and was then split into several sectors for modeling. The point sectors are: EGUs (ptegu), point source oil and gas extraction-related sources (pt_oilgas) and the remaining non-EGUs (ptnonipm). The EGU emissions are split out from the other sources to facilitate the use of distinct SMOKE temporal processing and future-year projection techniques. The oil and gas sector emissions (pt_oilgas) were processed separately for summary tracking purposes and distinct projection techniques from the remaining non-EGU emissions (ptnonipm).

The ptnonipm and pt_oilgas sector emissions were provided to SMOKE as annual emissions. The full description of how the NEI emissions were developed is provided in the NEI documentation, but a brief summary of their development follows:

a. CAP and HAP data were provided by States, locals and tribes under the Air Emissions Reporting Rule (AERR) [the reporting size threshold is larger for inventory years between the triennial inventory years of 2011, 2014, 2017, …]
b. EPA corrected known issues and filled PM data gaps.
c. EPA added HAP data from the Toxic Release Inventory (TRI) where corresponding data was not already provided by states/locals.
d. EPA stores and applies matches of the point source units to units with CEMS data and also for all EGU units modeled by EPA's Integrated Planning Model (IPM).
e. EPA provided data for airports and rail yards.
f. Off-shore platform data were added from the Bureau of Ocean Energy Management (BOEM).

The changes made to the NEI point sources prior to modeling with SMOKE are as follows:

- The tribal data, which do not use state/county Federal Information Processing Standards (FIPS) codes in the NEI, but rather use the tribal code, were assigned a state/county FIPS code of 88XXX, where XXX is the 3-digit tribal code in the NEI. This change was made because SMOKE requires all sources to have a state/county FIPS code.

- Sources that did not have specific counties assigned (i.e., the county code ends in 777) were not included in the modeling because it was only possible to know the state in which the sources resided, but no more specific details related to the location of the sources were available.

- Stack parameters for point sources missing this information were filled in prior to modeling in SMOKE.

Following the removal of point sources without specific locations (i.e., their FIPS code ends in 777), the point source FF10 was divided into three NEI-based platform point source sectors: the EGU sector (ptegu), point source oil and gas extraction-related emissions (pt_oilgas), and the remaining non-EGU sector also called the non-IPM (ptnonipm) sector. The split was done at the unit level for ptegu and facility level for pt_oilgas such that a facility may have units and processes in both ptnonipm and ptegu but, cannot be in both pt_oilgas and any other point sector.

The EGU emissions are split out from the other sources to facilitate the use of distinct SMOKE temporal processing and future-year projection techniques. The oil and gas sector emissions (pt_oilgas) were processed separately for summary tracking purposes and distinct future-year projection techniques from the remaining non-EGU emissions (ptnonipm).

For sources in the ptegu sector that could be matched to 2015 CEMS data, hourly CEMS NO_X and SO_2 emissions for 2015 from EPA's Acid Rain Program were used rather than annual inventory emissions. For all other pollutants (e.g., VOC, $PM_{2.5}$, HCl), annual emissions were used as-is from the annual inventory, but, were allocated to hourly values using heat input from the CEMS data. For the unmatched units in the ptegu sector, annual emissions were allocated to daily values using IPM region- and pollutant-specific profiles, and similarly, region- and pollutant-specific diurnal profiles were applied to create hourly emissions.

The inventory pollutants processed through SMOKE for all point source sectors were: carbon monoxide (CO), NO_X, VOC, sulfur dioxide (SO_2), ammonia (NH_3), particles less than 10 microns in diameter (PM_{10}), and particles less than 2.5 microns in diameter ($PM_{2.5}$), hydrochloric acid (HCl), and chlorine (Cl_2). The NBAFM species are explicit in the CB6-CMAQ chemical mechanism, but for point sources in the platform, these are generated through VOC speciation, as is normally done for non-toxics modeling applications. To prevent double counting of mass, NBAFM pollutants are dropped from the inventory by SMOKE. This is called the "no-integrate" VOC speciation case and is discussed in detail in Section 3.2.1.1.

Each of the point sectors is processed separately through SMOKE as described in the following subsections.

2.1.1 EGU sector (ptegu)

The ptegu sector contains emissions from EGUs in the 2015 point inventory that could be matched to units found in the National Electric Energy Data System (NEEDS) v5.16 database. The matching was prioritized according to the amount of the emissions produced by the source. In the SMOKE point flat file, emission records for sources that have been matched to the NEEDS database have a value filled into the IPM_YN column based on the matches stored within EIS.

Higher generation capacity units in the ptegu sector are matched to 2015 CEMS data from EPA's Clean Air Markets Division (CAMD) via ORIS facility codes and boiler ID. For the matched units, SMOKE replaces the 2015 emissions of NO_X and SO_2 with the CEMS emissions, thereby ignoring the annual values specified in the NEI. For other pollutants at matched units, the hourly CEMS heat input data are used to allocate the NEI annual emissions to hourly values. All stack parameters, stack locations, and Source Classification Codes (SCC) for these sources come from the NEI. Because these attributes are obtained from the NEI, the chemical speciation of VOC and $PM_{2.5}$ for the sources is selected based on the SCC or in some cases, based on unit-specific data. If CEMS data exists for a unit, but the unit is not matched to the NEI, the CEMS data for that unit is not used in the modeling platform. However, if the source exists in the NEI and is not matched to a CEMS unit, the emissions from that source are still modeled using the annual emission value in the NEI temporally allocated to hourly values. The EGU flat file inventory is split into a flat file with CEM matches and a flat file without CEM matches to support analysis and temporalization.

In the SMOKE point flat file, emission records for point sources matched to CEMS data have values filled into the ORIS_FACILITY_CODE and ORIS_BOILER_ID columns. The CEMS data in SMOKE-ready format is available at http://ampd.epa.gov/ampd/ near the bottom of the “Prepackaged Data” tab. Many smaller emitters in the CEMS program are not identified with ORIS facility or boiler IDs that can be matched to the NEI due to inconsistencies in the way a unit is defined between the NEI and CEMS datasets, or due to uncertainties in source identification such as inconsistent plant names in the two data systems. Also, the NEEDS database of units modeled by IPM includes many smaller emitting EGUs that do not have CEMS. Therefore, there will be more units in the NEEDS database than have CEMS data. The temporal allocation of EGU units matched to CEMS is based on the CEMS data, whereas regional profiles are used for most of the remaining units. More detail can be found in Section 3.3.2.

Some EIS units match to multiple CAMD units based on cross-reference information in the EIS alternate identifier table. The multiple matches are used to take advantage of hourly CEM data when a CAMD unit specific entry is not available in the inventory. Where a multiple match is made the EIS unit is split and the ORIS facility and boiler IDs are replaced with the individual CAMD unit IDs. The split EIS unit NOX and SO2 emissions annual emissions are replaced with the sum of CEM values for that respective unit. All other pollutants are scaled from the EIS unit into the split CAMD unit using the fraction of annual heat input from the CAMD unit as part of the entire EIS unit. The NEEDS ID in the “ipm_yn” column of the flat file is updated with a “_M_” between the facility and boiler identifiers to signify that the EIS unit had multiple CEMs matches.

For sources not matched to CEMS data, except for municipal waste combustors (MWC) waste-to-energy and cogeneration units, daily emissions were computed from the NEI annual emissions using average CEMS data profiles specific to fuel type, pollutant[2], and IPM region. To allocate emissions to each hour of the day, diurnal profiles were created using average CEMS data for heat input specific to fuel type and IPM region. See Section 3.3.2 for more details on the temporal allocation approach for ptegu sources. MWC and cogeneration units were specified to use uniform temporal allocation such that the emissions are allocated to constant levels for every hour of the year. These sources do not use hourly CEMs, and instead use a PTDAY file with the same emissions for each day, combined with a uniform hourly temporal profile applied by SMOKE

2.1.2 Point source oil and gas sector (pt_oilgas)

The pt_oilgas sector was separated from the ptnonipm sector by selecting sources with specific NAICS codes shown in Table 2-4. The emissions and other source characteristics in the pt_oilgas sector are submitted by states, while EPA developed a dataset of nonpoint oil and gas emissions for each county in the U.S. with oil and gas activity that was available for states to use. Nonpoint oil and gas emissions can be found in the np_oilgas sector. More information on the development of the 2014 oil and gas emissions can be found in Section 4.16 of the 2014NEIv2 TSD. The pt_oilgas sector includes emissions from offshore oil platforms.

Table 2-4. Point source oil and gas sector NAICS Codes

NAICS	NAICS description
2111,21111	Oil and Gas Extraction
211111	Crude Petroleum and Natural Gas Extraction
211112	Natural Gas Liquid Extraction
213111	Drilling Oil and Gas Wells
213112	Support Activities for Oil and Gas Operations

[2] The year to day profiles use NOx and SO_2 CEMS for NOx and SO_2, respectively. For all other pollutants, they use heat input CEMS data.

NAICS	NAICS description
2212, 22121, 221210	Natural Gas Distribution
4862,48621,486210	Pipeline Transportation of Natural Gas
48611, 486110	Pipeline Transportation of Crude Oil

The pt_oilgas inventory is a combination of sources with updated emissions for 2015, and sources with emissions carried forward from 2014NEIv2 with no updates. For this study, sources already updated for the year 2015 in EIS were used as-is. The emissions carried forward from 2014NEIv2 were projected to 2015. Projection factors for 2015 are based on historical state crude and natural gas production data from the U.S. Energy Information Administration (EIA), which is available at these two links: *http://www.eia.gov/dnav/ng/ng_sum_lsum_a_epg0_fgw_mmcf_a.htm*; *http://www.eia.gov/dnav/pet/pet_crd_crpdn_adc_mbbl_a.htm*. Separate factors are calculated for each state, and for sources related to oil production, gas production, or a combination of oil and gas. These factors, which are listed in Table 2-5, were applied to CO, NOx, and VOC emissions only from sources carried forward from the 2014NEIv2 pt_oilgas inventory. The table does not list every state; emissions in states that do not have projection factors listed were held constant. The complete 2015 pt_oilgas inventory used for this study consists of both sources already updated to 2015 within EIS (used directly), and sources carried forward from 2014NEIv2 (projected to 2015).

Table 2-5. Oil and gas sector 2015 projection factors

State	Oil projection factor	Gas projection factor	"Both" projection factor
Alabama	0.987	0.929	0.958
Alaska	0.973	1.002	0.988
Arizona	0.661	0.896	0.778
Arkansas	0.926	0.900	0.913
California	0.983	0.990	0.987
Colorado	1.284	1.028	1.156
Florida	0.991	1.822	1.407
Illinois	0.997	1.078	1.038
Indiana	0.885	1.096	0.990
Kansas	0.918	0.992	0.955
Kentucky	0.848	1.030	0.939
Louisiana	0.915	0.921	0.918
Maryland	1.000	1.900	1.900
Michigan	0.881	0.936	0.909
Mississippi	1.023	1.069	1.046
Missouri	0.760	0.333	0.547
Montana	0.955	0.984	0.970
Nebraska	0.950	1.144	1.047
Nevada	0.889	1.333	1.111
New Mexico	1.182	1.024	1.103
New York	0.798	0.858	0.828
North Dakota	1.088	1.262	1.175
Ohio	1.788	1.966	1.877
Oklahoma	1.121	1.072	1.097
Oregon	1.000	0.743	0.743

State	Oil projection factor	Gas projection factor	"Both" projection factor
Pennsylvania	1.034	1.130	1.082
South Dakota	0.927	0.948	0.937
Tennessee	0.897	0.808	0.852
Texas	1.089	1.016	1.053
Utah	0.908	0.917	0.913
Virginia	0.786	0.955	0.870
West Virginia	1.087	1.233	1.160
Wyoming	1.136	0.999	1.067

2.1.3 Non-IPM sector (ptnonipm)

With minor exceptions, the ptnonipm sector contains the point sources that are not in the ptegu or pt_oilgas sectors. For the most part, the ptnonipm sector reflects the non-EGU sources of the NEI point inventory; however, it is likely that some small low-emitting EGUs not matched to the NEEDS database or to CEMS data are present in the ptnonipm sector. The larger sources in this sector have 2015-specific emissions, while emissions for smaller sources that were not submitted for the 2015 NEI were pulled forward from the 2014NEIv2.

The ptnonipm sector contains a small amount of fugitive dust PM emissions from vehicular traffic on paved or unpaved roads at industrial facilities, coal handling at coal mines, and grain elevators. Sources with state/county FIPS code ending with "777" are in EIS but are not included in any modeling sectors. These sources typically represent mobile (i.e., temporary) asphalt plants that are only reported for some states and are generally in a fixed location for only a part of the year, and, are thus difficult to allocate to specific places and days as is needed for modeling. Therefore, these sources are dropped from the point-based sectors in the modeling platform.

2.2 Nonpoint sources (afdust, ag, agfire, ptagfire, np_oilgas, rwc, nonpt)

Several modeling platform sectors were created from the 2014NEIv2 nonpoint inventory. This section describes the *stationary* nonpoint sources. Locomotives, C1 and C2 CMV, and C3 CMV are also included the 2014NEIv2 nonpoint data category, but, are mobile sources that are described in Sections 2.4.1 and 2.4.2 as the cmv_c1c2, cmv_c3, and rail sectors. The 2014NEIv2 TSD, available from https://www.epa.gov/air-emissions-inventories/2014-national-emissions-inventory-nei-technical-support-document-tsd, includes documentation for the nonpoint sector of the 2014NEIv2.

The nonpoint tribal-submitted emissions are dropped during spatial processing with SMOKE due to the configuration of the spatial surrogates. This is to prevent possible double-counting with county-level emissions, and also because spatial surrogates for tribal data are not currently available. These omissions are not expected to have an impact on the results of the air quality modeling at the 12-km resolution used for this platform.

The following subsections describe how the sources in the 2014NEIv2 nonpoint inventory were separated into 2015 modeling platform sectors, along with any data that were replaced with non-NEI data or projected for 2015.

2.2.1 Area fugitive dust sector (afdust)

The area-source fugitive dust (afdust) sector contains PM_{10} and $PM_{2.5}$ emission estimates for nonpoint SCCs identified by EPA as dust sources. Categories included in the afdust sector are paved roads, unpaved roads and airstrips, construction (residential, industrial, road and total), agriculture production, and mining and quarrying. It does not include fugitive dust from grain elevators, coal handling at coal mines, or vehicular traffic on paved or unpaved roads at industrial facilities because these are treated as point sources so they are properly located.

The afdust sector is separated from other nonpoint sectors to allow for the application of a "transport fraction," and meteorological/precipitation reductions. These adjustments are applied using a script that applies land use-based gridded transport fractions, followed by another script that zeroes out emissions for hours on which at least 0.01 inches of precipitation occurs or there is snow cover on the ground. The land use data used to reduce the NEI emissions determines the amount of emissions that are subject to transport. This methodology is discussed in Pouliot, et al., 2010, and in "Fugitive Dust Modeling for the 2008 Emissions Modeling Platform" (Adelman, 2012). Both the transport fraction and meteorological adjustments are based on the gridded resolution of the platform (e.g., 12km grid cells); therefore, different emissions will result if the process were applied to different grid resolutions. A limitation of the transport fraction approach is the lack of monthly variability that would be expected with seasonal changes in vegetative cover. While wind speed and direction are not accounted for in the emissions processing, the hourly variability due to soil moisture, snow cover and precipitation is accounted for in the subsequent meteorological adjustment.

The sources in the afdust sector are for SCCs and pollutant codes (i.e., PM_{10} and $PM_{2.5}$) considered to be "fugitive" dust sources. These SCCs are provided in Table 2-6. Table 2-7 shows the SCCs that would have also been included in this sector if they had emissions in the 2014 NEI.

Table 2-6. SCCs in the afdust platform sector for NEI2014v2; nonzero emissions

SCC	SCC Description
2294000000	Mobile Sources;Paved Roads;All Paved Roads;Total: Fugitives
2294000002	Mobile Sources;Paved Roads;All Paved Roads;Total: Sanding/Salting - Fugitives
2296000000	Mobile Sources;Unpaved Roads;All Unpaved Roads;Total: Fugitives
2311000000	Industrial Processes;Construction: SIC 15 - 17;All Processes;Total
2311010000	Industrial Processes;Construction: SIC 15 - 17;Residential;Total
2311010070	Industrial Processes;Construction: SIC 15 - 17;Residential;Vehicle Traffic
2311020000	Industrial Processes;Construction: SIC 15 - 17;Industrial/Commercial/Institutional;Total
2311030000	Industrial Processes;Construction: SIC 15 - 17;Road Construction;Total
2325000000	Industrial Processes;Mining and Quarrying: SIC 14;All Processes;Total
2325060000	Industrial Processes;Mining and Quarrying: SIC 10;Lead Ore Mining and Milling;Total
2801000003	Miscellaneous Area Sources;Agriculture Production - Crops;Agriculture - Crops;Tilling
2801000005	Miscellaneous Area Sources;Agriculture Production - Crops;Agriculture - Crops;Harvesting
2801000007	Miscellaneous Area Sources;Agriculture Production - Crops;Agriculture - Crops;Loading
2801000008	Miscellaneous Area Sources;Agriculture Production - Crops;Agriculture - Crops;Transport

SCC	SCC Description
2805001000	Miscellaneous Area Sources; Agriculture Production - Livestock; Beef cattle - finishing operations on feedlots (drylots); Dust Kicked-up by Hooves (use 28-05-020, -001, -002, or -003 for Waste
2805001100	Miscellaneous Area Sources;Agriculture Production - Livestock;Beef cattle - finishing operations on feedlots (drylots);Confinement
2805001300	Miscellaneous Area Sources;Agriculture Production - Livestock;Beef cattle - finishing operations on feedlots (drylots);Land application of manure
2805002000	Miscellaneous Area Sources;Agriculture Production - Livestock;Beef cattle production composite;Not Elsewhere Classified
2805003100	Miscellaneous Area Sources;Agriculture Production - Livestock;Beef cattle - finishing operations on pasture/range;Confinement
2805007100	Miscellaneous Area Sources;Agriculture Production - Livestock;Poultry production - layers with dry manure management systems;Confinement
2805009100	Miscellaneous Area Sources;Agriculture Production - Livestock;Poultry production - broilers;Confinement
2805010100	Miscellaneous Area Sources;Agriculture Production - Livestock;Poultry production - turkeys;Confinement
2805018000	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle composite;Not Elsewhere Classified
2805020002	Miscellaneous Area Sources;Agriculture Production - Livestock;Cattle and Calves Waste Emissions;Beef Cows
2805023100	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle - drylot/pasture dairy;Confinement
2805030000	Miscellaneous Area Sources;Agriculture Production - Livestock;Poultry Waste Emissions;Not Elsewhere Classified (see also 28-05-007, -008, -009)
2805030007	Miscellaneous Area Sources;Agriculture Production - Livestock;Poultry Waste Emissions;Ducks
2805030008	Miscellaneous Area Sources;Agriculture Production - Livestock;Poultry Waste Emissions;Geese
2805035000	Miscellaneous Area Sources;Agriculture Production - Livestock;Horses and Ponies Waste Emissions;Not Elsewhere Classified
2805039100	Miscellaneous Area Sources;Agriculture Production - Livestock;Swine production - operations with lagoons (unspecified animal age);Confinement
2805040000	Miscellaneous Area Sources;Agriculture Production - Livestock;Sheep and Lambs Waste Emissions;Total
2805045000	Miscellaneous Area Sources;Agriculture Production - Livestock;Goats Waste Emissions;Not Elsewhere Classified
2805047100	Miscellaneous Area Sources;Agriculture Production - Livestock;Swine production - deep-pit house operations (unspecified animal age);Confinement
2805053100	Miscellaneous Area Sources;Agriculture Production - Livestock;Swine production - outdoor operations (unspecified animal age);Confinement

Table 2-7. SCCs in the afdust platform sector for NEI2014v2; zero emissions

SCC	SCC Description
2275085000	Mobile Sources; Aircraft; Unpaved Airstrips; Total
2801000000	Miscellaneous Area Sources; Agriculture Production - Crops; Agriculture - Crops; Total
2805001200	Miscellaneous Area Sources; Agriculture Production - Livestock; Beef cattle - finishing operations on feedlots (drylots); Manure handling and storage
2805007300	Miscellaneous Area Sources; Agriculture Production - Livestock; Poultry production - layers with dry manure management systems; Land application of manure
2805008100	Miscellaneous Area Sources; Agriculture Production - Livestock; Poultry production - layers with wet manure management systems; Confinement
2805008200	Miscellaneous Area Sources; Agriculture Production - Livestock; Poultry production - layers with wet manure management systems; Manure handling and storage
2805008300	Miscellaneous Area Sources; Agriculture Production - Livestock; Poultry production - layers with wet manure management systems; Land application of manure
2805009200	Miscellaneous Area Sources; Agriculture Production - Livestock; Poultry production - broilers; Manure handling and storage
2805009300	Miscellaneous Area Sources; Agriculture Production - Livestock; Poultry production - broilers; Land application of manure
2805010200	Miscellaneous Area Sources; Agriculture Production - Livestock; Poultry production - turkeys; Manure handling and storage
2805010300	Miscellaneous Area Sources; Agriculture Production - Livestock; Poultry production - turkeys; Land application of manure
2805019100	Miscellaneous Area Sources; Agriculture Production - Livestock; Dairy cattle - flush dairy; Confinement
2805019200	Miscellaneous Area Sources; Agriculture Production - Livestock; Dairy cattle - flush dairy; Manure handling and storage
2805019300	Miscellaneous Area Sources; Agriculture Production - Livestock; Dairy cattle - flush dairy; Land application of manure
2805021100	Miscellaneous Area Sources; Agriculture Production - Livestock; Dairy cattle - scrape dairy; Confinement
2805021200	Miscellaneous Area Sources; Agriculture Production - Livestock; Dairy cattle - scrape dairy; Manure handling and storage
2805021300	Miscellaneous Area Sources; Agriculture Production - Livestock; Dairy cattle - scrape dairy; Land application of manure
2805022100	Miscellaneous Area Sources; Agriculture Production - Livestock; Dairy cattle - deep pit dairy; Confinement
2805022200	Miscellaneous Area Sources; Agriculture Production - Livestock; Dairy cattle - deep pit dairy; Manure handling and storage
2805022300	Miscellaneous Area Sources; Agriculture Production - Livestock; Dairy cattle - deep pit dairy; Land application of manure
2805023200	Miscellaneous Area Sources; Agriculture Production - Livestock; Dairy cattle - drylot/pasture dairy; Manure handling and storage
2805023300	Miscellaneous Area Sources; Agriculture Production - Livestock; Dairy cattle - drylot/pasture dairy; Land application of manure
2805025000	Miscellaneous Area Sources; Agriculture Production - Livestock; Swine production composite; Not Elsewhere Classified (see also 28-05-039, -047, -053)
2805039200	Miscellaneous Area Sources; Agriculture Production - Livestock; Swine production - operations with lagoons (unspecified animal age); Manure handling and storage
2805039300	Miscellaneous Area Sources; Agriculture Production - Livestock; Swine production - operations with lagoons (unspecified animal age); Land application of manure

2805047300	Miscellaneous Area Sources; Agriculture Production - Livestock; Swine production - deep-pit house operations (unspecified animal age); Land application of manure

For the data compiled into the 2014NEIv2, meteorological adjustments are applied to paved and unpaved road SCCs but not transport adjustments. For the 2014NEIv1, the meteorological adjustments were inadvertently not applied. This created a large difference between the 2014NEIv1 and 2014NEIv2 dust emissions but did not impact the modeling platform. This is because the modeling platform applies meteorological adjustments and transport adjustments based on unadjusted NEI values (for both v1 and v2). For the 2014NEIv2, the meteorological adjustments that were applied (to paved and unpaved road SCCs) had to be backed out in order reapply them in SMOKE. Because it was determined that some counties in the v2 did not have the adjustment applied, their emissions were used as-is. Thus, the FF10 that is run through SMOKE consists of 100% unadjusted emissions, and after SMOKE all afdust sources have both transport and meteorological adjustments applied. The 2015 platform uses the same unadjusted afdust emissions inventory as the 2014v7.1 platform, except that meteorological adjustments are based on 2015 meteorology instead of 2014 meteorology.

The total impacts of the transport fraction and meteorological adjustments are shown in Table 2-8 after backing out the meteorological adjustment applied in the 2014NEIv2. The amount of the reduction ranges from about 92 percent in New Hampshire to about 23 percent in Nevada. The afdust emissions adjustments are similar to previous platforms. In the 2011v6.3 the reduction ranged from 29 percent in Nevada to 93 percent in New Hampshire.

Figure 2-1 illustrates the impact of each step of the adjustment, using the 2014v7.0 platform afdust sector as an example. The reductions due to the transport fraction adjustments alone are shown at the top of Figure 2-1. The reductions due to the precipitation adjustments are shown in the middle of Figure 2-1. The cumulative emission reductions after both transport fraction and meteorological adjustments are shown at the bottom of Figure 2-1. The top plot shows how the transport fraction has a larger reduction effect in the east, where forested areas are more effective at reducing PM transport than in many western areas. The middle plot shows how the meteorological impacts of precipitation, along with snow cover in the north, further reduce the dust emissions. These plots are from 2014; similar plots for 2015 would look slightly different depending on the meteorology for each year, but the general pattern would be the same.

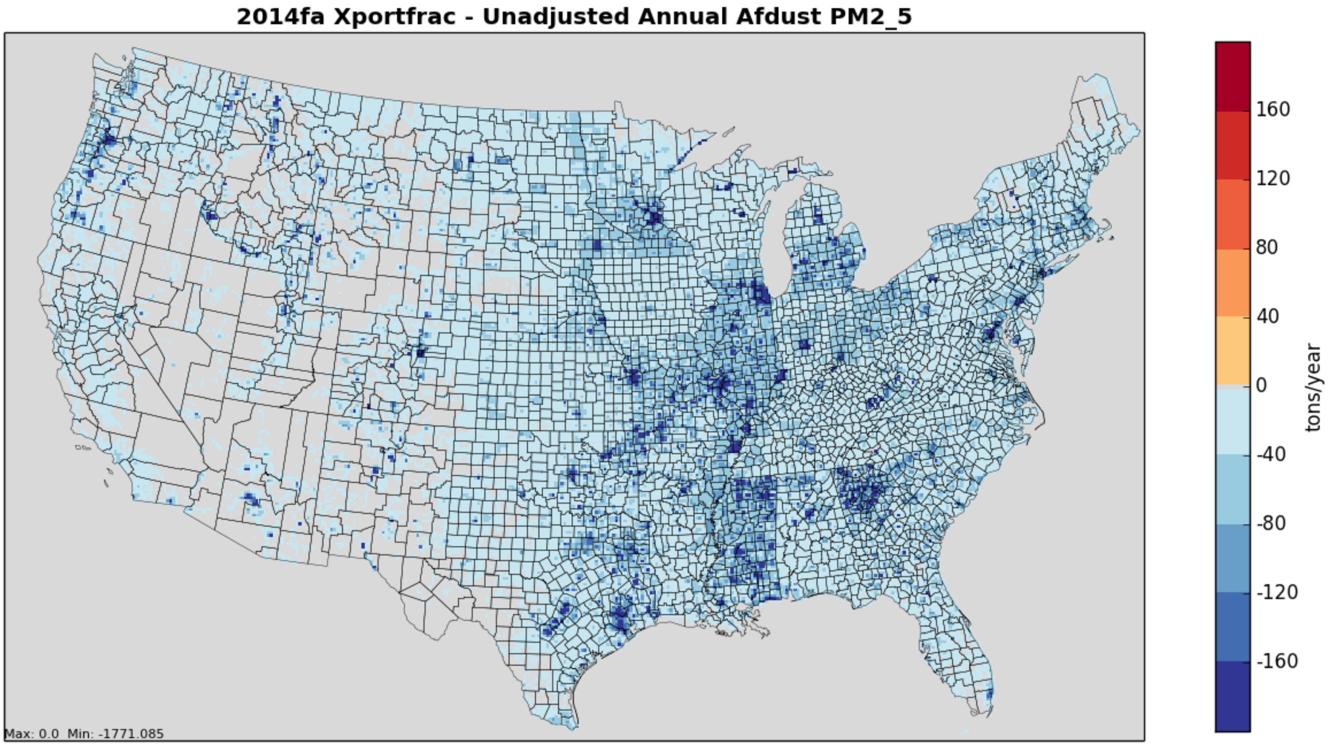
Table 2-8. Total impact of fugitive dust adjustments to unadjusted 2015 inventory

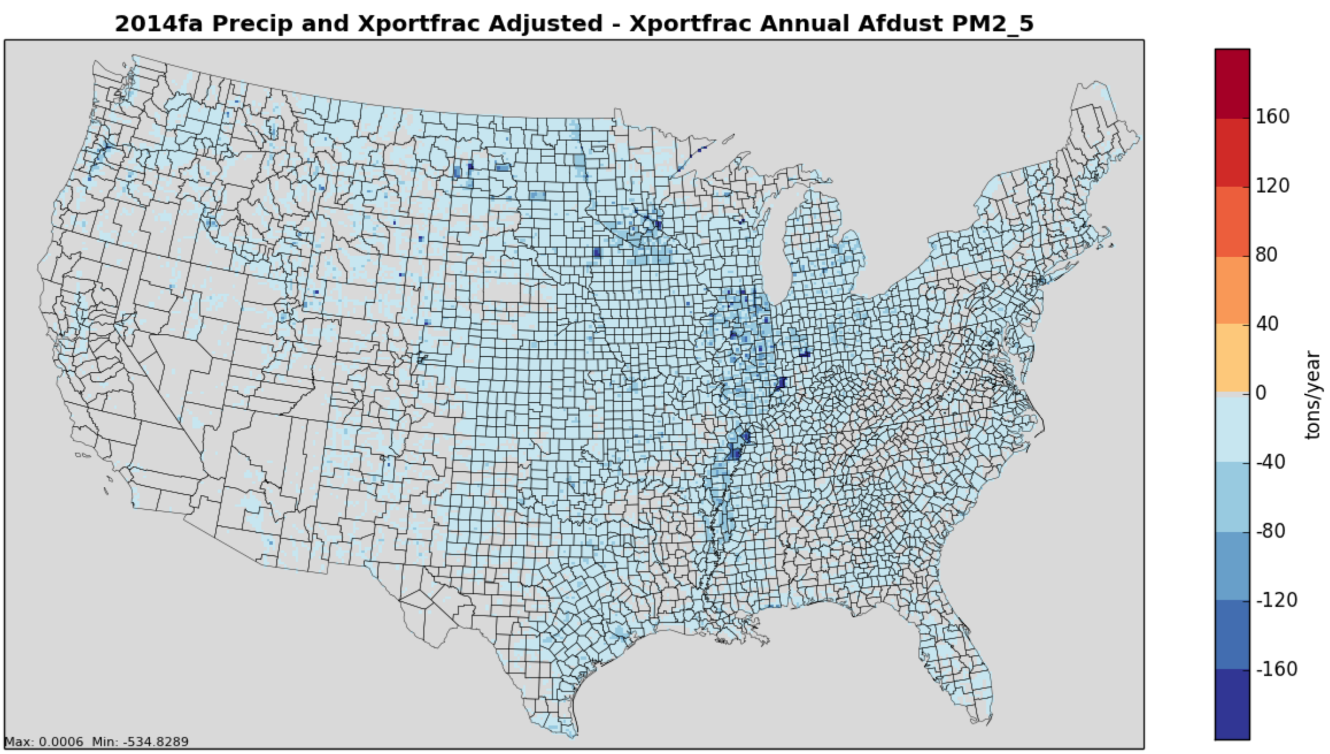
State	Unadjusted * PM_{10}	Unadjusted * $PM_{2.5}$	Change in PM_{10}	Change in $PM_{2.5}$	PM_{10} Reduction	$PM_{2.5}$ Reduction
Alabama	531,031	62,910	-442,078	-52,383	83%	83%
Arizona	263,092	32,550	-88,123	-10,861	33%	33%
Arkansas	319,532	49,024	-232,430	-34,783	73%	71%
California	312,541	41,065	-140,882	-18,105	45%	44%
Colorado	240,400	36,459	-145,182	-21,243	60%	58%
Connecticut	23,460	3,340	-20,134	-2,873	86%	86%
Delaware	14,318	2,456	-10,415	-1,791	73%	73%
District of Columbia	2,548	367.2044	-1,895	-272	74%	74%
Florida	715,123	81,227	-445,812	-50,405	62%	62%
Georgia	551,983	65,577	-460,090	-54,298	83%	83%

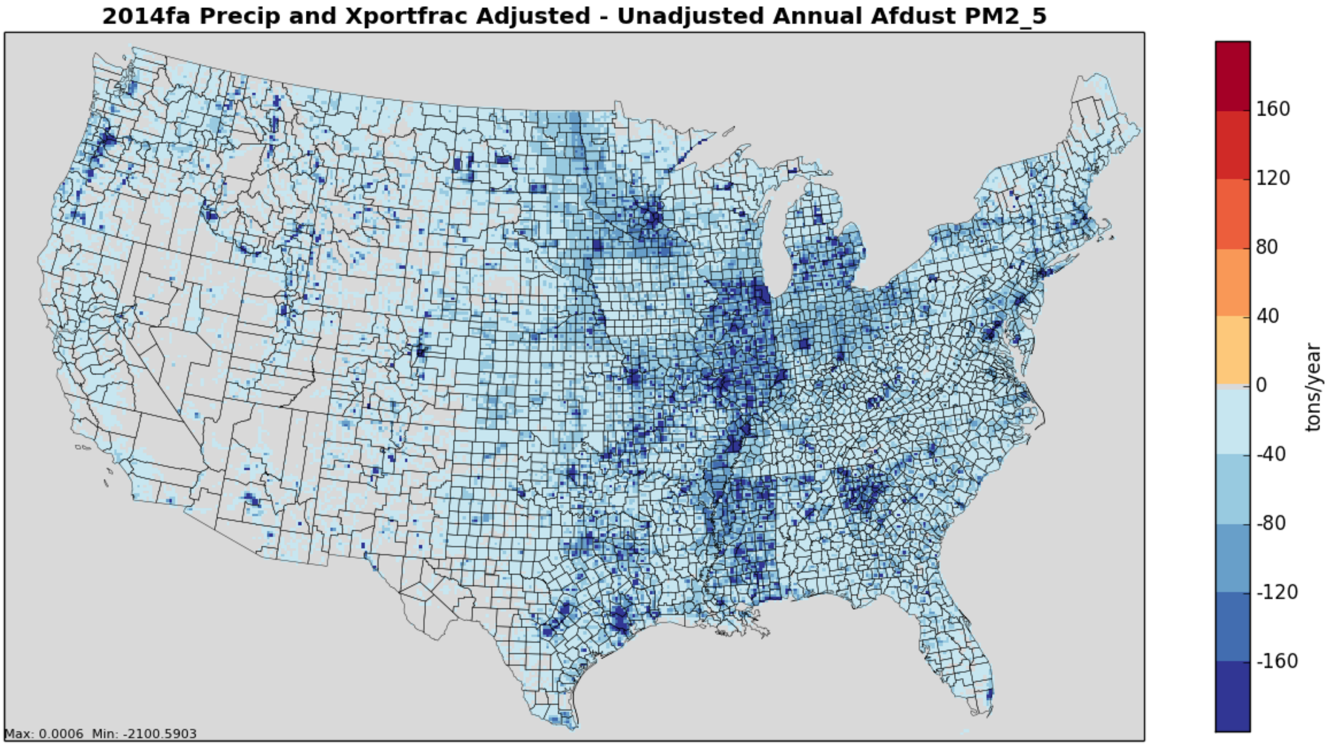
State	Unadjusted * PM_{10}	Unadjusted * $PM_{2.5}$	Change in PM_{10}	Change in $PM_{2.5}$	PM_{10} Reduction	$PM_{2.5}$ Reduction
Idaho	449,697	55,628	-287,356	-34,630	64%	62%
Illinois	994,459	143,538	-651,846	-93,806	66%	65%
Indiana	713,519	83,903	-517,070	-60,669	72%	72%
Iowa	384,930	59,847	-238,519	-37,058	62%	62%
Kansas	610,575	99,017	-304,968	-48,616	50%	49%
Kentucky	311,212	42,670	-249,008	-33,933	80%	80%
Louisiana	265,714	35,625	-194,577	-25,699	73%	72%
Maine	37,839	5,854	-33,368	-5,193	88%	89%
Maryland	103,187	16,226	-78,412	-12,310	76%	76%
Massachusetts	147,555	18,227	-123,552	-15,169	84%	83%
Michigan	388,475	48,399	-289,455	-35,891	75%	74%
Minnesota	403,298	61,415	-269,429	-40,598	67%	66%
Mississippi	432,447	53,220	-355,506	-43,106	82%	81%
Missouri	1,596,627	183,950	-1,200,402	-137,733	75%	75%
Montana	431,106	61,794	-255,652	-34,895	59%	56%
Nebraska	347,814	55,023	-184,530	-28,892	53%	53%
Nevada	159,219	22,770	-37,373	-5,208	23%	23%
New Hampshire	21,753	4,474	-19,969	-4,104	92%	92%
New Jersey	39,888	9,012	-30,798	-6,935	77%	77%
New Mexico	487,042	53,617	-179,264	-19,724	37%	37%
New York	266,547	44,918	-218,199	-36,801	82%	82%
North Carolina	201,722	29,165	-167,633	-24,298	83%	83%
North Dakota	472,493	82,404	-269,004	-46,732	57%	57%
Ohio	926,036	115,547	-698,919	-86,693	75%	75%
Oklahoma	448,835	67,558	-261,679	-38,509	58%	57%
Oregon	655,811	73,353	-494,124	-53,749	75%	73%
Pennsylvania	239,436	37,271	-200,011	-31,167	84%	84%
Rhode Island	4,774	758.9918	-3,599	-571	75%	75%
South Carolina	161,860	21,445	-127,773	-16,953	79%	79%
South Dakota	338,107	63,040	-188,679	-35,018	56%	56%
Tennessee	292,095	42,817	-237,706	-34,646	81%	81%
Texas	1,253,281	178,135	-693,229	-95,694	55%	54%
Utah	207,655	26,012	-104,611	-12,893	50%	50%
Vermont	22,127	3,211	-19,645	-2,842	89%	89%
Virginia	283,656	36,627	-239,498	-30,939	84%	84%
Washington	239,770	41,133	-136,452	-23,267	57%	57%
West Virginia	122,147	15,014	-111,989	-13,766	92%	92%
Wisconsin	687,446	89,364	-479,916	-62,117	70%	70%

State	Unadjusted * PM_{10}	Unadjusted * $PM_{2.5}$	Change in PM_{10}	Change in $PM_{2.5}$	PM_{10} Reduction	$PM_{2.5}$ Reduction
Wyoming	239,402	29,064	-127,537	-15,284	53%	53%
Domain Total	**18,363,585**	**2,486,019**	**-12,268,300**	**-1,633,119**	**67%**	**66%**
***** Unadjusted" here does not mean raw 2015, it means 2015 with met adjustments backed out as appropriate (i.e. the inventory that was fed into SMOKE)						

Figure 2-1. Impact of adjustments to 2014 fugitive dust emissions due to transport fraction, precipitation, and cumulative







2.2.2 Agricultural sector (ag)

The "ag" sector includes NH_3 emissions from fertilizer, and emissions of all pollutants other than $PM_{2.5}$ from livestock from 2014NEIv2, in the nonpoint (county-level) data category. $PM_{2.5}$ from livestock are in the afdust sector. The livestock and fertilizer emissions in this sector are based only on the SCCs starting with 2805. The livestock SCCs are related to beef and dairy cattle, poultry production and waste, swine production, waste from horses and ponies, and production and waste for sheep, lambs, and goats. Year 2014 ag sector emissions from the 2014NEIv2 were used as is for this 2015 study.

The fertilizer SCCs consist of 15 specific types of ammonia-based fertilizer and one for miscellaneous fertilizers. The "ag" sector includes all of the NH_3 emissions from fertilizer from the NEI. However, the "ag" sector does not include all of the livestock NH_3 emissions, as there is a very small amount of NH_3 emissions from livestock in the ptnonipm inventory (as point sources) in California (883 tons; less than 0.5 percent of state total) and Wisconsin (356 tons; about 1 percent of state total). In addition to NH_3, the "ag" sector also includes livestock emissions from all pollutants other than $PM_{2.5}$. Note that $PM_{2.5}$ from livestock are in the afdust sector.

Table 2-9 provides the SCCs for livestock. Of these, all have NH_3 and the ones marked in the 3rd column of the table include additional pollutants. Table 2-10 shows the fertilizer SCCs.

Table 2-9. Livestock SCCs extracted from the NEI to create the ag sector

SCC	SCC Description*	NH3+ other pollutants
2805001100	Beef cattle - finishing operations on feedlots (drylots);Confinement	
2805001200	Beef cattle - finishing operations on feedlots (drylots);Manure handling and storage	
2805001300	Beef cattle - finishing operations on feedlots (drylots);Land application of manure	Yes
2805002000	Beef cattle production composite; Not Elsewhere Classified	Yes
2805003100	Beef cattle - finishing operations on pasture/range; Confinement	
2805007100	Poultry production - layers with dry manure management systems;Confinement	Yes
2805007300	Poultry production - layers with dry manure management systems;Land application of manure	
2805008100	Poultry production - layers with wet manure management systems;Confinement	yes
2805008200	Poultry production - layers with wet manure management systems;Manure handling and storage	
2805008300	Poultry production - layers with wet manure management systems;Land application of manure	
2805009100	Poultry production - broilers;Confinement	yes
2805009200	Poultry production - broilers;Manure handling and storage	
2805009300	Poultry production - broilers;Land application of manure	
2805010100	Poultry production - turkeys;Confinement	yes
2805010200	Poultry production - turkeys;Manure handling and storage	yes
2805010300	Poultry production - turkeys;Land application of manure	
2805018000	Dairy cattle composite;Not Elsewhere Classified	yes
2805019100	Dairy cattle - flush dairy;Confinement	yes
2805019200	Dairy cattle - flush dairy;Manure handling and storage	
2805019300	Dairy cattle - flush dairy;Land application of manure	
2805020002	Cattle and Calves Waste Emissions:Beef Cows	
2805021100	Dairy cattle - scrape dairy;Confinement	yes
2805021200	Dairy cattle - scrape dairy;Manure handling and storage	
2805021300	Dairy cattle - scrape dairy;Land application of manure	
2805022100	Dairy cattle - deep pit dairy;Confinement	yes
2805022200	Dairy cattle - deep pit dairy;Manure handling and storage	
2805022300	Dairy cattle - deep pit dairy;Land application of manure	
2805023100	Dairy cattle - drylot/pasture dairy;Confinement	
2805023200	Dairy cattle - drylot/pasture dairy;Manure handling and storage	
2805023300	Dairy cattle - drylot/pasture dairy;Land application of manure	
2805025000	Swine production composite;Not Elsewhere Classified (see also 28-05-039, -047, -053)	yes
2805030000	Poultry Waste Emissions;Not Elsewhere Classified (see also 28-05-007, -008, -009)	yes
2805030007	Poultry Waste Emissions;Ducks	
2805030008	Poultry Waste Emissions;Geese	
2805035000	Horses and Ponies Waste Emissions;Not Elsewhere Classified	yes
2805039100	Swine production - operations with lagoons (unspecified animal age);Confinement	yes
2805039200	Swine production - operations with lagoons (unspecified animal age);Manure handling and storage	
2805039300	Swine production - operations with lagoons (unspecified animal age);Land application of manure	
2805040000	Sheep and Lambs Waste Emissions;Total	yes
2805045000	Goats Waste Emissions;Not Elsewhere Classified	yes
2805047100	Swine production - deep-pit house operations (unspecified animal age);Confinement	yes
2805047300	Swine production - deep-pit house operations (unspecified animal age);Land application of manure	
2805053100	Swine production - outdoor operations (unspecified animal age);Confinement	

* All SCC Descriptions begin “Miscellaneous Area Sources;Agriculture Production – Livestock”

Table 2-10. Fertilizer SCCs extracted from the NEI for inclusion in the "ag" sector

SCC	SCC Description*
2801700001	Anhydrous Ammonia
2801700002	Aqueous Ammonia
2801700003	Nitrogen Solutions
2801700004	Urea
2801700005	Ammonium Nitrate
2801700006	Ammonium Sulfate
2801700007	Ammonium Thiosulfate
2801700010	N-P-K (multi-grade nutrient fertilizers)
2801700011	Calcium Ammonium Nitrate
2801700012	Potassium Nitrate
2801700013	Diammonium Phosphate
2801700014	Monoammonium Phosphate
2801700015	Liquid Ammonium Polyphosphate
2801700099	Miscellaneous Fertilizers

* All descriptions include "Miscellaneous Area Sources; Agriculture Production – Crops; Fertilizer Application" as the beginning of the description.

Agricultural emissions in the platform are based on the 2014NEIv2, which is a mix of state-submitted data and EPA estimates. The EPA estimates in 2014NEIv2 were revised from 2014NEIv1, using refined methodologies and/or data for livestock and fertilizer. Livestock emissions utilized improved animal population data. VOC livestock emissions, new for this sector, were estimated by multiplying a national VOC/NH3 emissions ratio by the county NH3 emissions. The 2014NEI approach for livestock utilizes daily emission factors by animal and county from a model developed by Carnegie Mellon University (CMU) (Pinder, 2004, McQuilling, 2015) and 2012 and 2014 U.S. Department of Agriculture (USDA) agricultural census data. Details on the approach are provided in Section 4.5 of 2014NEIv2 TSD.

Annual fertilizer emissions were submitted by three states for all or part of the sector as shown in parentheses: California (57 percent), Illinois (100 percent) and Idaho (100 percent). Georgia had previously submitted data in v1 but used the EPA estimates for v2. The EPA estimates employed a methodology that uses the bidirectional (bi-di) version of CMAQ (v5.0.2) and the Fertilizer Emissions Scenario Tool for CMAQ FEST-C (v1.2). The FEST-C and CMAQ simulations were used to directly estimate emission rates based on 2014 inputs. This is a refinement from the earlier estimates that relied on emission factors calculated from a 2011 model simulation applied to 2014 FEST-C county level fertilizer application estimates. Additionally, revised FEST-C estimates of fertilizer application were reduced for pasture and hay due to estimates of fertilizer use and hay yield being higher than USDA estimates. This resulted in a reduction of NH_3 emissions, primarily in the Southeastern U.S. Section 4.5 of the 2014NEIv2 TSD presents the updated approach.

Agricultural emissions from livestock are based on the 2014NEIv2, which is a mix of state-submitted data and EPA estimates, and are unchanged from the 2014v7.1 platform. The EPA estimates in 2014NEIv2 were revised from 2014NEIv1, using refined methodologies and/or data. Livestock emissions utilized improved animal population data. VOC livestock emissions, new for this sector compared to the 2014v7.0 platform, were estimated by multiplying a national VOC/NH3 emissions ratio by the county NH3 emissions. HAP emissions used HAP-to-VOC factors from livestock profiles in the SPECIATE database (EPA, 2016). The 2014NEI approach for livestock utilizes daily emission factors by animal and county from a model developed by Carnegie Mellon University (CMU) (Pinder, 2004, McQuilling, 2015) and 2012 and 2014 U.S. Department of Agriculture (USDA) agricultural census data. Details on the approach are provided in Section 4.5 of the 2014NEIv1 TSD; updates for 2014NEIv2 (the new population estimates) are provided in Section 4.5 of the 2014NEIv2 TSD.

For livestock, meteorological-based temporal allocation (described in Section 3.3.5) is used for month-to-day and day-to-hour temporal allocation. Monthly profiles are based on the daily data underlying the EPA estimates. This was different from 2014v7.0 where the daily data underlying the NEI were used for generating daily emissions. Fertilizer uses different state-specific year-to-month profiles than livestock but uses the same meteorological-based month-to-hour profiles as livestock. These monthly profiles have not changed from previous platforms.

2.2.3 Agricultural fires (ptagfire)

In the NEI, agricultural fires are stored as county-annual emissions and are part of the nonpoint data category. For this study agricultural fires are modeled as day specific fires derived from satellite data for the year 2015, processed as point sources in support of CMAQ inline plume rise in a similar way to the emissions in ptfire, except with the sector name “ptagfire”. State-provided agricultural fire data from the 2014NEIv2 are not used in this study.

Heat flux and acres burned were provided by George Pouliot of EPA’s Office of Research and Development. Based on field reconnaissance of J. McCarty (2013, personal communication), a “typical” agricultural field size was assumed for each burn location, which varied by region of the country between 40 and 80 acres. The assumed field sizes can be found at http://www.epa.gov/sites/production/files/2015-06/draft_2014_ag_grasspasture_emissions_nei_may62015.xlsx. The heat flux calculation for each agricultural fire depends on estimated field size burned and the fuel loading by SCC (tons/acre). The fuel load estimate is also provided in the above spreadsheet. The ptagfire emissions estimated by the EPA are at point source and day-specific resolution. EPA data were developed using a multiple satellite detection database and crop level land use information. For the NEI, these are summed to the county and national level, but because they are computed at this finer temporal resolution, the more detailed data were used for this platform.

The agricultural fires sector includes SCCs starting with ‘28015’. The first three levels of descriptions for these SCCs are: 1) Fires - Agricultural Field Burning; Miscellaneous Area Sources; 2) Agriculture Production - Crops - as nonpoint; and 3) Agricultural Field Burning - whole field set on fire. The SCC 2801500000 does not specify the crop type or burn method, while the more specific SCCs specify field or orchard crops and, in some cases, the specific crop being grown. New agricultural field burning SCCs were added to the 2014 NEI to account for grass/pasture burning (also known as rangeland burning) which is included the agriculture field burning sector of the NEI.

For this modeling platform, a SMOKE update allows the use of HAP integration for speciation for PTDAY inventories. The 2015 agricultural fire inventory does not include emissions for HAPs, however, so this feature was not used for this study.

2.2.4 Nonpoint source oil and gas sector (np_oilgas)

The nonpoint oil and gas (np_oilgas) sector contains onshore and offshore oil and gas emissions. The EPA estimated emissions for all counties with 2014 oil and gas activity data with the Oil and Gas Tool, and many S/L/T agencies also submitted nonpoint oil and gas data. Where S/L/T submitted nonpoint CAPS but no HAPs, the EPA augmented the HAPs using HAP augmentation factors (county and SCC level) created from the Oil and Gas Tool. The types of sources covered include drill rigs, workover rigs, artificial lift, hydraulic fracturing engines, pneumatic pumps and other devices, storage tanks, flares, truck loading, compressor engines, and dehydrators. The SCCs that comprise this sector are listed in Appendix A.

The 2014NEIv2 nonpoint oil and gas inventory was projected to 2015 for this study. The methodology and projection factors for np_oilgas projections were the same as for pt_oilgas, except that 2015 projections were applied to the entire 2014NEIv2 np_oilgas inventory. Projection factors for 2015 are based on the same EIA crude and natural gas production data as the point oil and gas projections discussed in Section 2.1.2. Separate factors are calculated for each state, and for sources related to oil production, gas production, or a combination of oil and gas. These factors, which are listed in Table 2-5, were applied to CO, NOx, and VOC emissions from the 2014NEIv2 np_oilgas inventory.

2.2.5 Residential wood combustion sector (rwc)

The residential wood combustion (rwc) sector includes residential wood burning devices such as fireplaces, fireplaces with inserts (inserts), free standing woodstoves, pellet stoves, outdoor hydronic heaters (also known as outdoor wood boilers), indoor furnaces, and outdoor burning in firepits and chimneas. Free standing woodstoves and inserts are further differentiated into three categories: 1) conventional (not EPA certified); 2) EPA certified, catalytic; and 3) EPA certified, noncatalytic. Generally, the conventional units were constructed prior to 1988. Units constructed after 1988 had to meet EPA emission standards and they are either catalytic or non-catalytic. The SCCs in the rwc sector are listed in Table 2-11.

Residential wood combustion emissions for the 2015 platform are from 2014NEIv2. As with the other nonpoint categories, a mix of S/L and EPA estimates were used. The 2014NEIv2 EPA estimates included adjustments to appliance fractions to account for that not all appliances burn 100% wood (they also can burn natural gas and propane) and some changes to emission factors. For more information on the development of the residential wood combustion emissions, see Section 4.14 of the 2014NEIv2 TSD.

Table 2-11. SCCs in the residential wood combustion sector (rwc)*

SCC	SCC Description
2104008100	SSFC;Residential;Wood;Fireplace: general
2104008210	SSFC;Residential;Wood;Woodstove: fireplace inserts; non-EPA certified
2104008220	SSFC;Residential;Wood;Woodstove: fireplace inserts; EPA certified; non-catalytic
2104008230	SSFC;Residential;Wood;Woodstove: fireplace inserts; EPA certified; catalytic
2104008310	SSFC;Residential;Wood;Woodstove: freestanding, non-EPA certified
2104008320	SSFC;Residential;Wood;Woodstove: freestanding, EPA certified, non-catalytic
2104008330	SSFC;Residential;Wood;Woodstove: freestanding, EPA certified, catalytic
2104008400	SSFC;Residential;Wood;Woodstove: pellet-fired, general (freestanding or FP insert)
2104008510	SSFC;Residential;Wood;Furnace: Indoor, cordwood-fired, non-EPA certified
2104008610	SSFC;Residential;Wood;Hydronic heater: outdoor
2104008700	SSFC;Residential;Wood;Outdoor wood burning device, NEC (fire-pits, chimeas, etc)
2104009000	SSFC;Residential;Firelog;Total: All Combustor Types

* SSFC=Stationary Source Fuel Combustion

The spatial and temporal allocation for the rwc sector follow the same approach as in the 2014v7.1 platform. The temporal allocation of annual rwc emissions to day of year uses a meteorological-based approach for most SCCs as discussed in Section 3.3.4. For the 2015 platform, day-of-year temporalization is based on 2015 meteorology. All SCCs in this sector are spatially allocated using low intensity residential land (code 300).

2.2.6 Other nonpoint sources sector (nonpt)

Stationary nonpoint sources that were not subdivided into the afdust, ag, np_oilgas, or rwc sectors were assigned to the "nonpt" sector. Locomotives and CMV mobile sources from the 2014NEIv2 nonpoint inventory are not included in this sector and are described in Section 2.4.1. There are too many SCCs in the nonpt sector to list all of them individually, but the types of sources in the nonpt sector include:

- stationary source fuel combustion, including industrial, commercial, and residential and orchard heaters;
- commercial sources such as commercial cooking;
- industrial processes such as chemical manufacturing, metal production, mineral processes, petroleum refining, wood products, fabricated metals, and refrigeration;
- solvent utilization for surface coatings such as architectural coatings, auto refinishing, traffic marking, textile production, furniture finishing, and coating of paper, plastic, metal, appliances, and motor vehicles;
- solvent utilization for degreasing of furniture, metals, auto repair, electronics, and manufacturing;
- solvent utilization for dry cleaning, graphic arts, plastics, industrial processes, personal care products, household products, adhesives and sealants;
- solvent utilization for asphalt application and roofing, and pesticide application;
- storage and transport of petroleum for uses such as portable gas cans, bulk terminals, gasoline service stations, aviation, and marine vessels;
- storage and transport of chemicals;
- waste disposal, treatment, and recovery via incineration, open burning, landfills, and composting;
- miscellaneous area sources such as cremation, hospitals, lamp breakage, and automotive repair shops.

The nonpt sector includes emission estimates for Portable Fuel Containers (PFCs), also known as "gas cans." The PFC inventory consists of five distinct sources of PFC emissions, further distinguished by residential or commercial use. The five sources are: (1) displacement of the vapor within the can; (2) spillage of gasoline while filling the can; (3) spillage of gasoline during transport; (4) emissions due to evaporation (i.e., diurnal emissions); and (5) emissions due to permeation. Note that spillage and vapor displacement associated with using PFCs to refuel nonroad equipment are included in the nonroad inventory.

For the 2015 platform, the emissions inventory for the nonpt sector is from 2014NEIv2 and is the same as in the 2014v7.1 platform.

2.3 Onroad mobile sources (onroad)

Onroad mobile source emissions result from motorized vehicles that are normally operated on public roadways. These include passenger cars, motorcycles, minivans, sport-utility vehicles, light-duty trucks, heavy-duty trucks, and buses. The sources are further divided between diesel, gasoline, E-85, and compressed natural gas (CNG) vehicles. The sector characterizes emissions from parked vehicle processes (e.g., starts, hot soak, and extended idle) as well as from on-network processes (i.e., from vehicles as they move along the roads). Except for California, all onroad emissions are generated using the SMOKE-MOVES emissions modeling framework that leverages MOVES generated emission factors (http://www.epa.gov/otaq/models/moves/index.htm), county and SCC-specific activity data, and hourly meteorological data.

The onroad SCCs in the modeling platform are more resolved than those in the NEI, because the NEI SCCs distinguish vehicles and fuels, but in the platform, they also distinguish between off-network, extended idle, and the various MOVES road-types. For more details on the approach and for a summary of the inputs submitted by states, see the section 6.5 of the 2014NEIv2 TSD. The 2015 platform includes emission factors processed by MOVES for the year 2015, and projections of 2014NEIv2 vehicle miles traveled, vehicle population, and hoteling (extended idling) hours activity data to 2015.

2.3.1 Onroad (onroad)

For the continental U.S., the EPA uses a modeling framework that accounts for the temperature sensitivity of the on-road emissions. Specifically, the EPA used MOVES inputs for representative counties, vehicle miles traveled (VMT), vehicle population (VPOP), and hoteling data for all counties, along with tools that integrated the MOVES model with SMOKE. In this way, it was possible to take advantage of the gridded hourly temperature information available from meteorology modeling used for air quality modeling. The "SMOKE-MOVES" integration tool was originally developed by the EPA in 2010 and is used for regional air quality modeling of onroad mobile sources.

SMOKE-MOVES requires that emission rate "lookup" tables be generated by MOVES, which differentiates emissions by process (i.e., running, start, vapor venting, etc.), vehicle type, road type, temperature, speed, hour of day, etc. To generate the MOVES emission rates that could be applied across the U.S., the EPA used an automated process to run MOVES to produce emission factors for a series of temperatures and speeds for a set of "representative counties," to which every other county is mapped. Representative counties are used because it is impractical to generate a full suite of emission factors for the more than 3,000 counties in the U.S. The representative counties for which emission factors are generated are selected according to their state, elevation, fuels, age distribution, ramp fraction, and inspection and maintenance programs. Each county is then mapped to a representative county based on its similarity to the representative county with respect to those attributes. For age distributions and vehicle fuel types, rather than choose the value based on the representative county, a weighted average was computed. For the 2015 platform, there are 303 representative counties, same as in the 2014v7.1 platform. A detailed discussion of the representative counties is in the 2014NEIv2 TSD, Section 6.8.2.

Once representative counties have been identified, emission factors are generated by running MOVES for each representative county and for two "fuel months" – January to represent winter months, and July to represent summer months – because different types of fuels are used in each season. SMOKE selects the appropriate MOVES emissions rates for each county, hourly temperature, SCC, and speed bin and multiplies the emission rate by appropriate activity data: VMT (vehicle miles travelled), VPOP (vehicle population), or HOTELING (hours of extended idle) to produce emissions. These calculations are done for every county and grid cell in the continental U.S. for each hour of the year.

The SMOKE-MOVES process for creating the model-ready emissions consists of the following steps:

1) Determine which counties will be used to represent other counties in the MOVES runs.
2) Determine which months will be used to represent other month's fuel characteristics.

3) Create inputs needed only by MOVES. MOVES requires county-specific information on vehicle populations, age distributions, speed distribution, temporal profiles, and inspection-maintenance programs for each of the representative counties.
4) Create inputs needed both by MOVES and by SMOKE, including temperatures and activity data.
5) Run MOVES to create emission factor tables for the temperatures and speeds that exist in each county during the modeled period.
6) Run SMOKE to apply the emission factors to activity data (VMT, VPOP, and HOTELING) to calculate emissions based on the gridded hourly temperatures in the meteorological data.
7) Aggregate the results to the county-SCC level for summaries and QA.

The onroad emissions are processed in four processing streams that are merged together into the onroad sector emissions after each of the four streams have been processed:

- rate-per-distance (RPD) uses VMT as the activity data plus speed and speed profile information to compute on-network emissions from exhaust, evaporative, permeation, refueling, and brake and tire wear processes;
- rate-per-vehicle (RPV) uses VPOP activity data to compute off-network emissions from exhaust, evaporative, permeation, and refueling processes;
- rate-per-profile (RPP) uses VPOP activity data to compute off-network emissions from evaporative fuel vapor venting, including hot soak (immediately after a trip) and diurnal (vehicle parked for a long period) emissions; and
- rate-per-hour (RPH) uses hoteling hours activity data to compute off-network emissions for idling of long-haul trucks from extended idling and auxiliary power unit process.

The list of emission modes and SCCs differ between the platform and the NEI. Both SMOKE-MOVES runs were generated at the same level of detail, but the NEI emissions were aggregated into 2 all-inclusive modes: refueling and all other modes. In addition, the NEI SCCs were aggregated over roads to all parking and all road emissions. The list of modes (or aggregate processes) and the corresponding MOVES processes mapped to them are listed in Table 2-12.

Table 2-12. Onroad emission aggregate processes

Aggregate process	Description	MOVES process IDs
40	All brake and tire wear	9;10
53	All extended idle exhaust	17;90
62	All refueling	18;19
72	All exhaust and evaporative except refueling and hoteling	1;2;11;12;13;15;16
91	Auxiliary Power Units	91

The onroad emissions inputs for the platform are based on the 2014NEIv2, described in more detail in Section 6 of the 2014NEIv2 TSD. These inputs include:

- MOVES County databases (CDBs) including Low Emission Vehicle (LEV) table
- Representative counties
- Fuel months
- Meteorology

- Activity data (VMT, VPOP, speed, HOTELING)

Representative counties and fuel months are the same as for the 2014NEIv2, while other inputs were updated for the year 2015. The activity data was projected from 2014 to 2015 using the following procedure. First, VMT was projected using factors calculated from FHWA VM-2 data (https://www.fhwa.dot.gov/policyinformation/statistics/2014/vm2.cfm, https://www.fhwa.dot.gov/policyinformation/statistics/2015/vm2.cfm). Year-to-year projection factors were calculated by state, with separate factors for urban and rural road types, and then applied to the 2014NEIv2 VMT. In some states, a single state-wide projection factor for all road types was computed, usually in states with large discrepancies in how activity is split between urban and rural road types in the FHWA data as compared to the 2014NEIv2 VMT dataset. States for which a single projection factor was applied state-wide are: Alaska, Georgia, Indiana, Louisiana, Maine, Massachusetts, Nebraska, New Mexico, New York, North Dakota, Tennessee, Virginia, and West Virginia. Furthermore, in Texas and Utah, a single state-wide projection factor was calculated based on state-wide VMT totals provided by each state's Department of Transportation[3]. VMT projection factors for all states are shown in Table 2-13.

Table 2-13. Factors applied to project VMT from 2014 to 2015

State	Rural roads	Urban roads
Alabama	2.28%	2.53%
Alaska	3.89%	3.89%
Arizona	0.31%	5.02%
Arkansas	2.59%	2.54%
California	2.36%	0.51%
Colorado	2.02%	3.36%
Connecticut	1.24%	1.29%
Delaware	4.42%	3.08%
District of Columbia	0.00%	0.84%
Florida	4.17%	2.73%
Georgia	5.89%	5.89%
Hawaii	3.50%	0.78%
Idaho	1.57%	5.32%
Illinois	1.32%	-0.01%
Indiana	-0.49%	-0.49%
Iowa	4.36%	7.29%
Kansas	0.82%	3.45%
Kentucky	1.66%	1.39%
Louisiana	-0.15%	-0.15%
Maine	2.29%	2.29%
Maryland	2.01%	1.90%

[3] Sources of Texas data: https://ftp.dot.state.tx.us/pub/txdot-info/trf/crash_statistics/2014/01.pdf, https://ftp.dot.state.tx.us/pub/txdot-info/trf/crash_statistics/2015/01.pdf
Sources of Utah data: https://www.udot.utah.gov/main/uconowner.gf?n=32396326443209656, https://www.udot.utah.gov/main/uconowner.gf?n=27035817009129993

State	Rural roads	Urban roads
Massachusetts	2.96%	2.96%
Michigan	2.80%	-0.49%
Minnesota	0.00%	0.00%
Mississippi	-1.35%	4.08%
Missouri	1.50%	1.37%
Montana	1.22%	2.29%
Nebraska	2.49%	2.49%
Nevada	3.70%	2.17%
New Hampshire	1.25%	0.76%
New Jersey	3.00%	0.56%
New Mexico	8.24%	8.24%
New York	-1.57%	-1.57%
North Carolina	2.92%	3.91%
North Dakota	-4.52%	-4.52%
Ohio	1.43%	0.54%
Oklahoma	1.51%	-1.12%
Oregon	6.06%	2.70%
Pennsylvania	-1.44%	2.47%
Rhode Island	1.32%	2.12%
South Carolina	4.30%	3.01%
South Dakota	1.23%	0.72%
Tennessee	5.99%	5.99%
Texas	6.23%	6.23%
Utah	6.62%	6.62%
Vermont	4.50%	1.47%
Virginia	2.02%	2.02%
Washington	3.91%	2.30%
West Virginia	3.71%	3.71%
Wisconsin	3.68%	3.03%
Wyoming	1.74%	0.88%
Puerto Rico	0.00%	0.00%
Virgin Islands	0.00%	0.00%

Once the VMT dataset was finalized for 2015, VPOP activity for 2015 was calculated by applying VMT/VPOP ratios based on 2014NEIv2 to the projected 2015 VMT for each county, fuel, and vehicle type. Hoteling hours activity for 2015 were calculated in a similar manner, by applying 2014NEIv2-based VMT/hoteling ratios to the projected 2015 VMT, but only for VMT from long-haul combination trucks on restricted roads.

An additional step was taken for the refueling emissions. Colorado submitted point emissions for refueling for some counties[4]. For these counties, the EPA zeroed out the onroad estimates of refueling (i.e., SCCs =220xxxxx62) so that the states' point emissions would take precedence. The onroad refueling emissions were zeroed out using the adjustment factor file (CFPRO) and Movesmrg.
For more detailed information on the methods used to develop the 2014 onroad mobile source emissions and the input data sets, see the 2014NEIv2 TSD.

California is the only state agency for which submitted onroad emissions were used in the 2014 NEIv2 and 2015 platform. California uses their own emission model, EMFAC, which uses emission inventory codes (EICs) to characterize the emission processes instead of SCCs. The EPA and California worked together to develop a code mapping to better match EMFAC's EICs to EPA MOVES' detailed set of SCCs that distinguish between off-network and on-network and brake and tire wear emissions. This detail is needed for modeling but not for the NEI. This code mapping is provided in "2014v1_EICtoEPA_SCCmapping.xlsx." which is found in the supporting data for the 2014 NEI v2 TSD (ftp://newftp.epa.gov/air/nei/2014/doc/2014v2_supportingdata/onroad/). California provided their CAP and HAP emissions by county using EPA SCCs after applying the mapping. There was one change made after the mapping: the vehicle/fuel type combination gas intercity buses (first 6 digits of the SCC = 220141), that is not generated using MOVES, was changed to gasoline single unit short-haul trucks (220152) for consistency with the modeling inventory. California provided EMFAC2014-based onroad emissions inventories for 2014 and 2017; emissions inventories from those two years were interpolated to 2015 values for this platform.

The California onroad mobile source emissions were created through a hybrid approach of combining state-supplied annual emissions with EPA-developed SMOKE-MOVES runs. Through this approach, the platform was able to reflect the unique rules in California, while leveraging the more detailed SCCs and the highly resolved spatial patterns, temporal patterns, and speciation from SMOKE-MOVES. The basic steps involved in temporally allocating onroad emissions from California based on SMOKE-MOVES results were:

1) Run CA using EPA inputs through SMOKE-MOVES to produce hourly 2015 emissions hereafter known as "EPA estimates." These EPA estimates for CA are run in a separate sector called "onroad_ca."
2) Calculate ratios between state-supplied emissions and EPA estimates[5]. These were calculated for each county/SCC/pollutant combination. Unlike in previous platforms, the California data separated off and on-network emissions and extended idling. However, the on-network did not provide specific road types, and California's emissions did not include information for vehicles fueled by E-85, so these differentiations were obtained using MOVES.
3) Create an adjustment factor file (CFPRO) that includes EPA-to-state estimate ratios.
4) Rerun CA through SMOKE-MOVES using EPA inputs and the new adjustment factor file.

Through this process, adjusted model-ready files were created that sum to annual totals from California, but have the temporal and spatial patterns reflecting the highly resolved meteorology and SMOKE-MOVES. After adjusting the emissions, this sector is called "onroad_ca_adj." Note that in emission

[4] There were 52 counties in Colorado that had point emissions for refueling. Outside Colorado, it was determined that refueling emissions in the 2014 NEIv2 point did not significantly duplicate the refueling emissions in onroad.
[5] These ratios were created for all matching pollutants. These ratios were duplicated for all appropriate modeling species. For example, the EPA used the NO_X ratio for NO, NO_2, HONO and used the $PM_{2.5}$ ratio for PEC, PNO_3, POC, PSO_4, etc. (For more details on NO_X and PM speciation, see Sections 3.2.2, and 3.2.3. For VOC model-species, the EPA used VOC ratios.)

summaries, the emissions from the “onroad” and “onroad_ca_adj” sectors are summed and designated as the emissions for the onroad sector.

2.4 2014 nonroad mobile sources (cmv, rail, nonroad)

The nonroad mobile source emission modeling sectors consist of nonroad equipment emissions (nonroad), locomotive (rail) and CMV emissions.

2.4.1 Category 1, Category 2, Category 3 Commercial Marine Vessels (cmv_c1c2, cmv_c3)

The cmv_c1c2 and cmv_c3 sectors contain commercial marine vessel (CMV) emissions. The cmv_c1c2 sector contains Category 1 and 2 (C1 and C2) CMV emissions that traverse state and Federal waters and that are in the 2014 NEIv2. The cmv_c3 sector contains Category 3 emissions that traverse state and Federal waters (in the NEI) plus C3 in waters not covered by the NEI. The C1 and C2 emissions were split from C3 to allow the C3 to be modeled as point sources with plume rise.

All NEI emissions from these sectors that are in state waters are annual and at county-SCC resolution; however, in the NEI they are provided at the sub-county level (port or underway shape ids) and by SCC and emission type (e.g., hoteling, maneuvering). NEI emission estimates are a mix of state-submitted values and EPA-developed emissions in areas where states did not submit. The emissions developed by EPA use a “bottom up” procedure based on activity details from the U.S. Coast Guard and Army Corps of Engineers databases. For the 2014NEIv2, emissions developed by the Lake Michigan Air Directors Consortium (LADCO) were used for several states in the region: Illinois, Indiana, Iowa, Minnesota, Michigan, Missouri, Ohio and Wisconsin. In addition, Delaware submitted data for v2. See section 4.19 of the 2014NEIv2 TSD for a description of the methodology and updates to commercial marine vessels in the 2014NEIv2.

The NEI includes CMV outside of state waters, but that are in Federal waters (FIPS = 85). These areas include parts of the Gulf of Mexico and East and West Coasts. The U.S. Federal waters around Puerto Rico and Alaska are outside the CONUS modeling domain and are not used in the platform. The Federal Waters emissions are also categorized as port or underway shapes.

For the 2015 platform, cmv_c1c2 emissions from the 2014NEIv2 were used as-is. In a future 2015 study, SO_2 emissions were reduced by 90% from 2014NEIv2 levels in accordance with ECA-IMO emissions standards for 2016, but this reduction was not applied in this 2015 study.

Table 2-14 provides the SCCs extracted from the NEI for the cmv_c1c2 sector. For the purpose of the NEI, it is assumed that C1 and C2 vessels typically used distillate fuels.

Table 2-14. SCCs extracted for the cmv_c1c2 sector

SCC	Sector	Description: Mobile Sources prefix for all
2280002100	cmv	Marine Vessels; Commercial; Diesel; Port
2280002200	cmv	Marine Vessels; Commercial; Diesel; Underway

The sources in the cmv_c1c2 sector are gridded from the county estimates. For the 2015 platform, ports for c1/c2 use a surrogate based on Ports NEI2014 activity (surrogate 820), and underway emissions use a surrogate based on 2013 shipping density (surrogate 808).

Table 2-15 provides the SCCs extracted from the NEI for the cmv_c3 sector. For the purpose of the NEI, it is assumed that C3 vessels typically use residual blends; however, in California, the larger C3 vessels are required to use cleaner diesel fuel in state waters and were thus mapped to C1 and C2 vessels. In the future, these SCCs will change to properly categorize C3 vessels that use diesel fuel appropriately.

Table 2-15. SCCs extracted for the cmv_c3 sector

SCC	Sector	Description: Mobile Sources prefix for all
2280003100	cmv	Marine Vessels, Commercial; Residual; Port emissions
2280003200	cmv	Marine Vessels, Commercial; Residual; Underway emissions

The cmv_c3 sector sources are treated as point sources. This allows plume rise to be computed so that emissions can be allocated to air quality model layers higher than layer 1. A set of fixed stack parameters were assigned to every CMV point source: 65.62 ft (20 m) height, 2.625 ft (0.8 m) diameter, 82.02 ft/s (25 m/s) velocity and 539.5 F (282 C).

The 2015 platform C3 emissions are from 2014NEIv2 within U.S. state and federal waters (FIPS = 85). In a future 2015 study, SO_2 emissions in the cmv_c3 sector were reduced by 90% from 2014NEIv2 levels within state and federal waters, in accordance with ECA-IMO emissions standards for 2016. However, this SO_2 cut was not applied for this 2015 study.

The “ECA-IMO-based” C3 CMV inventory is used for waters not covered by the NEI (with FIPS assigned to 98001) and is used for allocating the county-level NEI emissions to geographic locations. These data are described below.

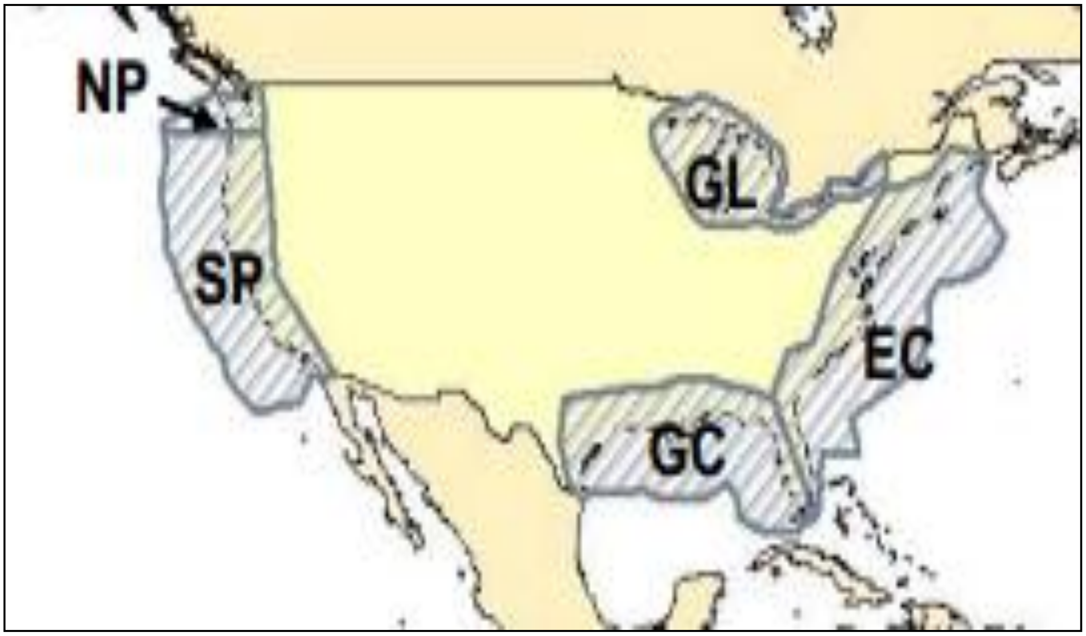
The EPA-“ECA-IMO-based” emissions were developed based on a 4-km resolution ASCII raster format dataset that preserves shipping lanes. This dataset has been used since the ECA-IMO project began in 2005, although it was then known as the Sulfur Emissions Control Area (SECA). The ECA-IMO emissions consist of large marine diesel engines (at or above 30 liters/cylinder) that, until recently, were allowed to meet relatively modest emission requirements and, as a result, these ships would often burn residual fuel in that region. The emissions in this sector are comprised of primarily foreign-flagged ocean-going vessels, referred to as C3 CMV ships. The cmv inventory sector includes these ships in several intra-port modes (i.e., cruising, hoteling, reduced speed zone, maneuvering, and idling) and an underway mode, and includes near-port auxiliary engine emissions.

An overview of the C3 ECA Proposal to the International Maritime Organization project (EPA-420-F-10-041, August 2010) and future-year goals for reduction of NO_X, SO_2, and PM C3 emissions can be found at: http://www.epa.gov/oms/regs/nonroad/marine/ci/420r09019.pdf. The resulting ECA-IMO coordinated strategy, including emission standards under the Clean Air Act for new marine diesel engines with per-cylinder displacement at or above 30 liters, and the establishment of ECA is available from http://www.epa.gov/oms/oceanvessels.htm. The base-year ECA inventory is 2002 and consists of these CAPs: PM_{10}, $PM_{2.5}$, CO, CO_2, NH_3, NO_X, SO_X (assumed to be SO_2), and hydrocarbons (assumed to be VOC). The EPA developed regional growth (activity-based) factors that were applied to create the 2011 inventory from the 2002 data. These growth factors are provided in Table 2-16. The geographic regions listed in the table are shown in Figure 2-2. The East Coast and Gulf Coast regions were divided along a line roughly through Key Largo (longitude 80° 26’ West). Technically, the Exclusive Economic Zone (EEZ) FIPS are not really “FIPS” state-county codes, but are treated as such in the inventory and emissions processing.

Table 2-16. Growth factors to project the 2002 ECA-IMO inventory to 2011

Region	EEZ FIPS	NO_X	PM_{10}	$PM_{2.5}$	VOC	CO	SO_2
Outside ECA	98001	1.341	1.457	1.457	1.457	1.457	1.457

Figure 2-2. Illustration of regional modeling domains in ECA-IMO study



The emissions were converted to SMOKE point source inventory format as described in http://www3.epa.gov/ttn/chief/conference/ei17/session6/mason.pdf, allowing for the emissions to be allocated to modeling layers above the surface layer. As described in the paper, the ASCII raster dataset was converted to latitude-longitude, mapped to state/county FIPS codes that extended up to 200 nautical miles (nm) from the coast, assigned stack parameters, and monthly ASCII raster dataset emissions were used to create monthly temporal profiles. All non-US, non-EEZ emissions (i.e., in waters considered outside of the 200 nm EEZ and, hence, out of the U.S. and Canadian ECA-IMO controllable domain) were simply assigned a dummy state/county FIPS code=98001 and were projected to year 2011 using the "Outside ECA" factors in Table 2-16.

No data from this inventory were used for State waters which extend approximately 3 to 10 miles offshore or FIPs beginning with 85, since these were taken from the 2014NEIv2. However, the "ECA-IMO-based" inventory was used to convert the NEI emissions to point sources. Also, the SMOKE-ready data have been cropped from the original ECA-IMO entire northwestern quarter of the globe to cover only the large continental U.S. 36-km "36US3" air quality model domain, the largest Continental U.S. domain used by the EPA in recent years. Emissions in Canadian Federal waters are also removed from the ECA-IMO-based inventory to prevent a double count with a separate C3 emissions inventory provided by Environment Canada.

The original ECA-IMO inventory did not delineate between ports and underway emissions (or other C3 modes such as hoteling, maneuvering, reduced-speed zone, and idling). However, a U.S. ports spatial surrogate dataset was used to assign the ECA-IMO emissions to ports and underway SCCs 2280003100 and 2280003200, respectively. This had no effect on temporal allocation or speciation because all C3 CMV emissions, unclassified/total, port and underway, share the same temporal and speciation profiles. See Section 3.2.1.2 for more details on C3 speciation in the cmv sector and Section 3.3.8 for details on temporal allocation.

A hierarchical process was used for generating the geographic coordinates of the points. The ECA inventory was used as a first choice, port polygons as a next choice (for port SCCs), and then gridding surrogates where there is not county overlap between the C3 emissions and the ECA or port polygons.

2.4.2 Railroad sources: (rail)

The rail sector includes all locomotives in the NEI nonpoint data category, SCCs are shown in Table 2-17. This sector excludes railway maintenance locomotives and point source yard locomotives. Railway maintenance emissions are included in the nonroad sector. The point source yard locomotives are included in the ptnonipm sector.

The nonpoint rail data, which for 2015 platform are unchanged from those in the 2014NEIv2, are a mix of S/L and EPA data. EPA estimates cover only SCCs 2285002006 and 2285002007. Revised and/or new data were provided by some states for the 2014NEIv2 as compared to the 2014NEIv1. The EPA data were completely replaced from the v1 estimates, which had been carried forward from the 2011 NEI. The updated EPA data were developed by the Eastern Regional Technical Advisory Committee's (ERTAC) rail group. The group coordinated with the Federal Rail Administration to collect link-based activity data and apply the equipment-specific emission factors appropriate. For more information on locomotive sources in the NEI, see Section 4.20 of the 2014NEIv2 TSD.

Table 2-17. 2014NEIv2 SCCs extracted for rail sector

SCC	Sector	Description: Mobile Sources prefix for all
2285002006	rail	Railroad Equipment;Diesel;Line Haul Locomotives: Class I Operations
2285002007	rail	Railroad Equipment;Diesel;Line Haul Locomotives: Class II / III Operations
2285002008	rail	Railroad Equipment;Diesel;Line Haul Locomotives: Passenger Trains (Amtrak)
2285002009	rail	Railroad Equipment;Diesel;Line Haul Locomotives: Commuter Lines
2285002010	rail	Railroad Equipment;Diesel;Yard Locomotives

2.4.3 Nonroad mobile equipment sources: (nonroad)

The nonroad equipment emissions in the platform and the NEI result primarily from running the MOVES2014a model, which incorporates the NONROAD2008 model. MOVES2014a replaces NMIM, which was used for 2011 and earlier NEIs. MOVES2014a provides a complete set of HAPs and incorporates updated nonroad emission factors for HAPs. MOVES2014a was used for all states other than California, which uses their own model. Additional details on the development of the 2014NEI nonroad emissions are available in Section 5 of the 2014NEIv2 TSD. The basis of nonroad emissions in the 2015 platform is an interpolation of emissions from separate runs of MOVES2014a for 2014 and 2016. The 2016 run of MOVES2014a that was used for this interpolation was found to not be a true representation of 2016 emissions and instead represented year 2014 emissions with 2016 meteorology, therefore the nonroad emissions are representative of year 2014 instead of 2015. This was corrected in a later version of year 2015 inventories.

The magnitude of the annual emissions in the nonroad inventory used here are similar to the emissions in the nonroad data category of the 2014NEIv2. Unlike the NEI, the platform has monthly emission totals, which are provided by MOVES2014a, and contain additional pollutants used in the emissions modeling. The emissions in the modeling platform include NONHAPTOG and ETHANOL, and these are not included in the NEI. NONHAPTOG is the difference between total organic gases (TOG) and explicit species that are estimated separately such as benzene, toluene, styrene, ethanol, and numerous other compounds and are integrated into the chemical speciation process. MOVES2014a provides estimates of NONHAPTOG along with the speciation profile code for the NONHAPTOG emission source. This is accomplished by using NHTOG#### as the pollutant code in the FF10 inventory file, where #### is a speciation profile code. Since speciation profiles are applied by SCC and pollutant, no changes to SMOKE were needed to use the FF10 with this profile information. This approach is not used for California, because their model provides VOC and traditional speciation is performed instead.

Nonroad emissions for California submitted to NEI were developed using the California Emissions Projection Analysis Model (CEPAM) that supports various California off-road regulations. Documentation of the CARB offroad mobile methodology, including CMV sector data, is provided at: http://www.arb.ca.gov/msei/categories.htm#offroad_motor_vehicles. The CARB-supplied nonroad annual inventory emissions values were temporalized to monthly values using monthly temporal profiles applied in SMOKE by SCC. Some VOC emissions were added to California to account for situations when VOC HAP emissions were included in the inventory, but VOC emissions were either less than the sum of the VOC HAP emissions, or were missing entirely. These additional VOC emissions were computed by summing benzene, acetaldehyde, formaldehyde, and naphthalene for the specific sources. California nonroad inventories were available for years 2014 and 2017; emissions for those two years were interpolated to 2015 values for this platform.

2.5 "Other Emissions": non-U.S. sources

The emissions from Canada and Mexico are included as part of five emissions modeling sectors: othpt, othar, othafdust, onroad_can, and onroad_mex. The "oth" refers to the fact that these emissions are usually "other" than those in the NEI, and the remaining characters provide the SMOKE source types: "pt" for point, "ar" for "area and nonroad mobile," "afdust" for area fugitive dust (Canada only). Because Canada and Mexico onroad mobile emissions are modeled differently from each other, they are separated into two sectors: onroad_can and onroad_mex.

2.5.1 Point sources from Canada and Mexico (othpt)

For Canadian point sources, 2013 and 2025 emissions provided by Environment Canada were interpolated to year 2015 for facilities included in both the 2013 and 2025 datasets. Sources that were only in the 2013 dataset and not in 2025 (i.e. closures) were omitted from the 2016 dataset. Sources that were only in the 2025 dataset and not in 2013 (i.e. newly opened facilities) were included in the 2015 inventory with emissions set to 2025 values, except for the Bonnybrook Energy Centre facility in Alberta, which as of 2018 has not opened and thus was left out of the 2015 inventory. These Canadian point source inventories included VOC emissions with CB6 speciation, although the CB6 VOCs differed slightly from the version of CB6 in CMAQ. Environment Canada also provided total unspeciated VOC, which was added to the inventory as VOC_INV and was speciated for ACET, CH4 and CB6-CMAQ species not covered in the CB6-speciated inventory (XYLMN, NAPH and SOAALK). Airport emissions were provided by month. Temporal profiles were provided for all source categories. Other than the CB6 species of NBAFM present in the speciated NPRI data, there are no explicit HAP emissions in this inventory.

Point sources in Mexico were compiled based on inventories projected from the the Inventario Nacional de Emisiones de Mexico, 2008 (ERG, 2017). The point source emissions were converted to English units and into the FF10 format that could be read by SMOKE, missing stack parameters were gapfilled using SCC-based defaults, and latitude and longitude coordinates were verified and adjusted if they were not consistent with the reported municipality. Mexican point inventories were projected from 2008 to the years 2014 and 2018, and then those emissions values were interpolated to the year 2016 for this platform. Only CAPs are included in the Mexico point source inventory.

2.5.2 Area and nonroad mobile sources from Canada and Mexico (othar, othafdust)

For Canadian area and nonroad sources, year-2013 emissions provided by Environment Canada were used for this 2015 study, including CMV emissions for most pollutants. A later 2015 study recomputed Canadian emissions based on an interpolation of 2013 and 2025 emissions, but for this 2015 study, the 2013 emissions were used directly. Agricultural ammonia and nonroad emissions inventories from Canada are monthly; rail, CMV and other nonpoint Canada sectors are annual. The following Canadian area inventories are sub-province: agricultural ammonia (for all provinces) and nonroad (Quebec, Ontario, and BC only). The ag inventory goes all the way down to census division. For nonroad, Quebec/Ontario/BC resolution is by “region”, not by census division, with only a couple of regions in each province.

The Canadian inventory included fugitive dust emissions that do not incorporate either a transportable fraction or meteorological-based adjustments. To properly account for this, a separate sector called othafdust was created and modeled using the same adjustments as are done for U.S. sources (see Section 2.2.1 for more details). Updated Shapefiles used for creating spatial surrogates for Canada were also provided.

For Mexican area and nonroad sources, emission projections based on Mexico’s 2008 inventory were used for area and nonroad sources (ERG, 2017). The resulting inventory was written using English units to the nonpoint FF10 format that could be read by SMOKE. Note that unlike the U.S. inventories, there are no explicit HAPs in the nonpoint or nonroad inventories for Canada and Mexico and, therefore, all HAPs are created from speciation. Similar to the point inventories, Mexican area and nonroad inventories were projected from 2008 to the years 2014 and 2018, and then emissions values were interpolated to year 2015 values for this platform.

2.5.3 Onroad mobile sources from Canada and Mexico (onroad_can, onroad_mex)

For Canada onroad emissions, month-specific year-2013 emissions provided by Environment Canada were used for this year 2015 study. This inventory is sub-province in Ontario (4 regions) and BC (2 regions), and province elsewhere. There are no explicit HAPs in the onroad inventories for Canada, and therefore, NBAFM HAPs are created from speciation.

For Mexico onroad emissions, a version of the MOVES model for Mexico was run that provided the same VOC HAPs and speciated VOCs as for the U.S. MOVES model (ERG, 2016a). This includes NBAFM plus several other VOC HAPs such as toluene, xylene, ethylbenzene and others. Except for VOC HAPs that are part of the speciation, no other HAPs are included in the Mexico onroad inventory (such as particulate HAPs nor diesel particulate matter). Mexico onroad inventories were generated by MOVES for the years 2014 and 2017, and then emissions values were interpolated to the year 2015 for this platform.

2.5.4 Fires from Canada and Mexico (*ptfire_othna*)

Annual 2015 wildland emissions for Mexico, Canada, Central America, and Caribbean nations in the 2015 platform were developed from a combination of FINN (Fire Inventory from NCAR) daily fire emissions and fire data provided by Environment Canada when available. Environment Canada emissions were used for Canada wildland fire emissions for April through November and FINN fire emissions were used to fill in the annual gaps from January through March and December. Only CAP emissions are provided in the ptfire_othna sector inventories.

For FINN fires, listed vegetation type codes of 1 and 9 are defined as agricultural burning, all other fire detections and assumed to be wildfires. All wildland fires that are not defined as agricultural are assumed to be wild fires rather than prescribed. FINN fire detects less than 50 square meters (0.012 acres) are removed from the inventory. The locations of FINN fires are geocoded from latitude and longitude to FIPS code.

2.6 Fires (ptfire)

Wildfire and prescribed burning emissions are contained in the ptfire sector. The ptfire sector has emissions provided at geographic coordinates (point locations) and has daily emissions values. The ptfire sector excludes agricultural burning and other open burning sources that are included in the ptagfire sector. Emissions are day-specific and include satellite-derived latitude/longitude of the fire's origin and other parameters associated with the emissions such as acres burned and fuel load, which allow estimation of plume rise.

The ptfire sector excludes agricultural burning and other open burning sources that are included in the nonpt sector. The NEI SCCs for the ptfire sector are shown in Table 2-18.

Table 2-18. 2014 Platform SCCs representing emissions in the ptfire modeling sector

SCC	SCC Description*
2810001001	Other Combustion-as Event; Forest Wildfires; Smoldering
2810001002	Other Combustion-as Event; Forest Wildfires; Flaming
2811015001	Other Combustion-as Event; Prescribed Forest Burning; Smoldering
2811015002	Other Combustion-as Event; Prescribed Forest Burning; Flaming

* The first tier level of the SCC Description is "Miscellaneous Area Sources."

The point source day-specific emission estimates for 2015 fires were developed using SMARTFIRE 2 (Sullivan, et al., 2008), which uses the National Oceanic and Atmospheric Administration's (NOAA's) Hazard Mapping System (HMS) fire location information as input. Additional inputs include the CONSUME v4.1 software application (Joint Fire Science Program, 2009) and the Fuel Characteristic Classification System (FCCS) fuel-loading database to estimate fire emissions from wildfires and prescribed burns on a daily basis. The method involves the reconciliation of ICS-209 reports (Incident Status Summary Reports), GeoMAC perimeter Shapefiles, USFS fire information, and USFWS fire information data with satellite-based fire detections to determine spatial and temporal information about the fires. A functional diagram of the SMARTFIRE 2 process of reconciling fires with ICS-209 reports is available in the documentation (Raffuse, et al., 2007). Once the fire reconciliation process is completed, the emissions are calculated using the U.S. Forest Service's CONSUME v4.1 fuel consumption model and the FCCS v2 fuel-loading database in the BlueSky Framework (Ottmar, et. al., 2007).

A difference between the fires for this study and those in the NEI is that the proportion of emissions allocated to flaming versus smoldering SCCs were adjusted. Flaming fractions were calculated for each fire based on the flaming and smoldering consumption divided by the total consumption. Smoldering fractions were calculated by dividing the residual consumption by the total consumption. The fractions were then applied to the 2015 fire emissions to obtain revised emissions for the flaming and smoldering SCCs. The total emissions by state were unchanged, but they were reapportioned to the flaming and smoldering SCCs to facilitate a more realistic plume rise for fires.

Large fires of more than 20,000 acres in a single day were split using GeoMAC (https://www.geomac.gov/) fire shapes, where available, or otherwise using a circle centered on the detect lat/lon based on 12US2 grid cell overlap. The resulting split fires have emissions and area apportioned from the original fire into the grid cells based on fraction of area overlap between the fire shape and the cell. The idea is to prevent all of the emissions from a very large fire from going into a single grid cell, when in reality the fire emissions were more dispersed than a single point. The area of each of the "subfires" was computed in proportion to the overlap with that grid cell. These "subfires" were given new names that were the same as the original, but with "_a", "_b", "_c", and "_d" appended as needed.

The SMOKE-ready inventory files created from the raw daily fires contain both CAPs and HAPs. The BAFM HAP emissions from the inventory were obtained using VOC speciation profiles (i.e., a "no-integrate noHAP" use case).

2.7 Biogenic sources (beis)

Biogenic emissions were developed using the Biogenic Emission Inventory System version 3.61 (BEIS3.61) within SMOKE using the "15j" version of 2015 meteorology. BEIS3.61 creates gridded, hourly, model-species emissions from vegetation and soils. It estimates CO, VOC (most notably isoprene, terpene, and sesquiterpene), and NO emissions for the contiguous U.S. and for portions of Mexico and Canada. Biogenic emissions can be processed within SMOKE (the "offline" option), or within CMAQ using the same inputs as SMOKE (the "inline" option). For this platform, the offline option was used for CMAQ modeling, and so the model-ready emissions input to CMAQ include biogenics.

For the 2014NEIv2, land use changes were made for the states of Florida, Texas and Washington to correct an error with the land use fractions which did not sum to 1; but the version remained named BELD4.1. The same land use version is used for this platform.

The BEIS3.61 was used in conjunction with the modified Version 4.1 of the Biogenic Emissions Landuse Database (BELD4) and incorporates a canopy two-layer canopy model to estimate leaf-level temperatures (Pouliot and Bash, 2015). In the BEIS 3.61 two-layer canopy model, the layer structure varies with light intensity and solar zenith angle. Both layers include estimates of sunlit and shaded leaf area based on solar zenith angle and light intensity, direct and diffuse solar radiation, and leaf temperature (Bash et al., 2015). The new algorithm requires additional meteorological variables over previous versions of BEIS. The variables output from the Meteorology-Chemistry Interface Processor (MCIP) that are used to convert WRF outputs to CMAQ inputs are shown in Table 2-19.

Table 2-19. Meteorological variables required by BEIS 3.61

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

The BELD version 4.1 is based on an updated version of the USDA-USFS Forest Inventory and Analysis (FIA) vegetation speciation based data from 2001 to 2014 from the FIA version 5.1. Canopy coverage is based on the Landsat satellite National Land Cover Database (NLCD) product from 2011. The FIA includes approximately 250,000 representative plots of species fraction data that are within approximately 75 km of one another in areas identified as forest by the NLCD canopy coverage. The 2011 NLCD provides land cover information with a native data grid spacing of 30 meters. For land areas outside the conterminous United States, 500 meter grid spacing land cover data from the Moderate Resolution Imaging Spectroradiometer (MODIS) is used. BELDv4.1 also incorporates the following:

- 30 meter NASA's Shuttle Radar Topography Mission (SRTM) elevation data (http://www2.jpl.nasa.gov/srtm/) to more accurately define the elevation ranges of the vegetation species than in previous versions; and
- 2011 30 meter USDA Cropland Data Layer (CDL) data (http://www.nass.usda.gov/research/Cropland/Release/).

For the 2014NEIv2 and this study, land use changes were made for the states of Florida, Texas and Washington to correct an error with the land use fractions which did not sum to 1; but the version remained named BELD4.1.

Biogenic emissions computed with BEIS version 3.61 were left out of the CMAQ-ready merged emissions, in favor of inline biogenics produced during the CMAQ model run itself.

To provide a sense of the scope and spatial distribution of the emissions, plots of annual BEIS outputs for NO, isoprene, acetaldehyde, and formaldehyde associated with the 2014v7.0 platform are shown in Figure 2-3, Figure 2-4, Figure 2-5, and Figure 2-6, respectively. The land use changes made in the v7.1 platform would not impact these v7.0-based figures. The biogenic emissions for 2015 are different from 2014 in terms of temporalization and magnitude but, are similar spatially.

Figure 2-3. Annual NO emissions output from BEIS 3.61 for 2014

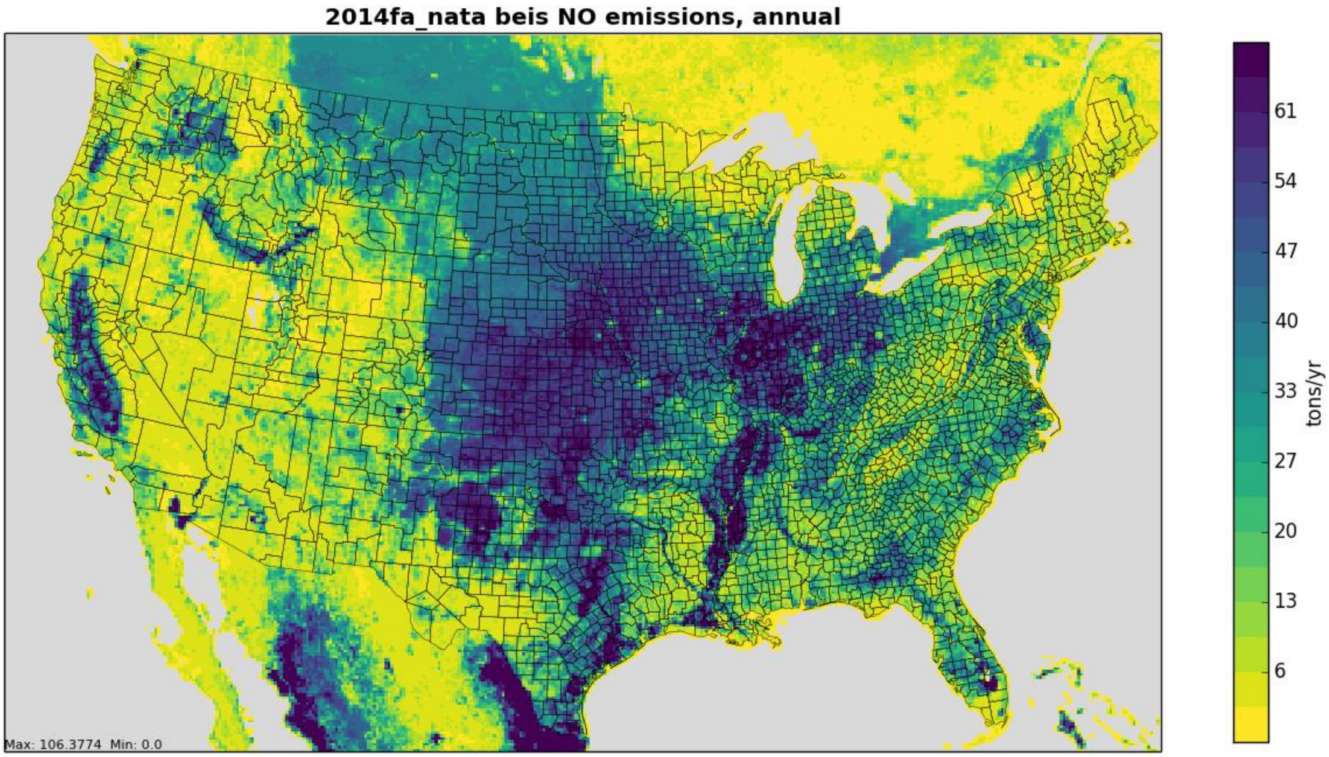


Figure 2-4. Annual isoprene emissions output from BEIS 3.61 for 2014

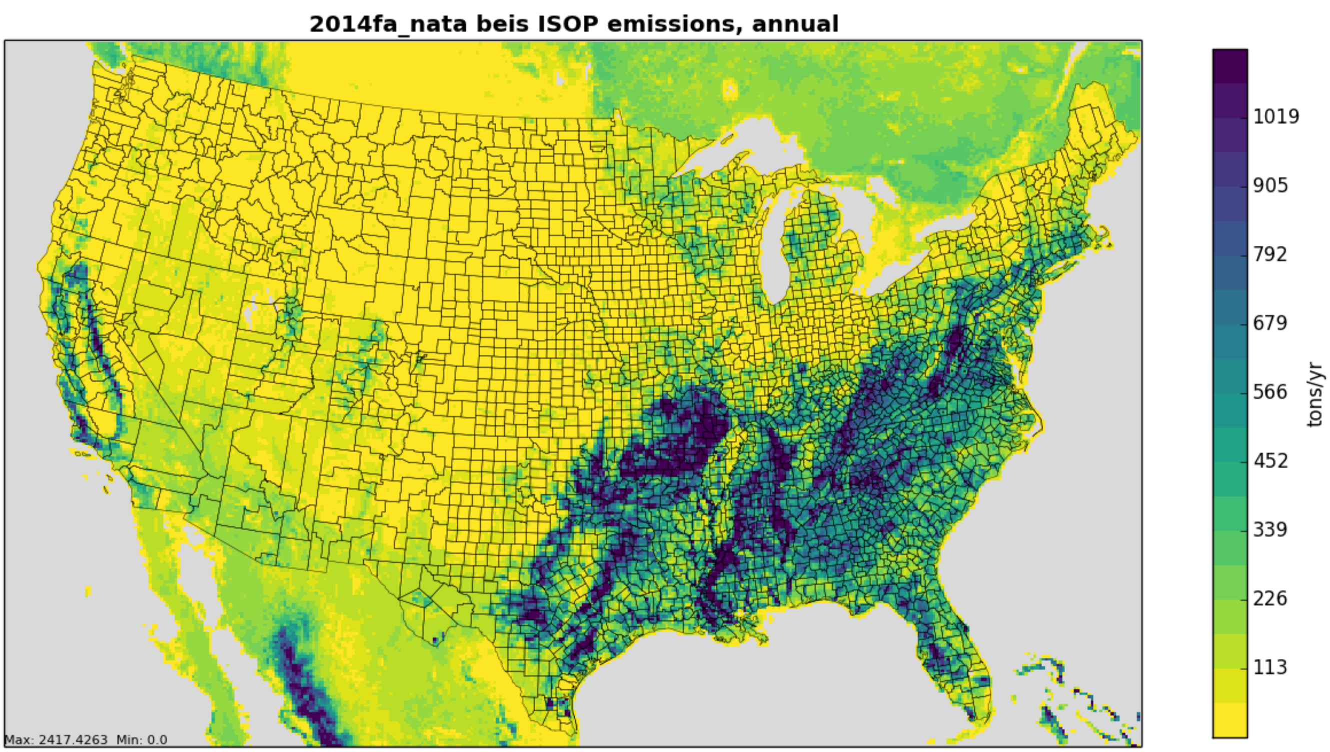


Figure 2-5. Annual acetaldehyde emissions output from BEIS 3.61 for 2014

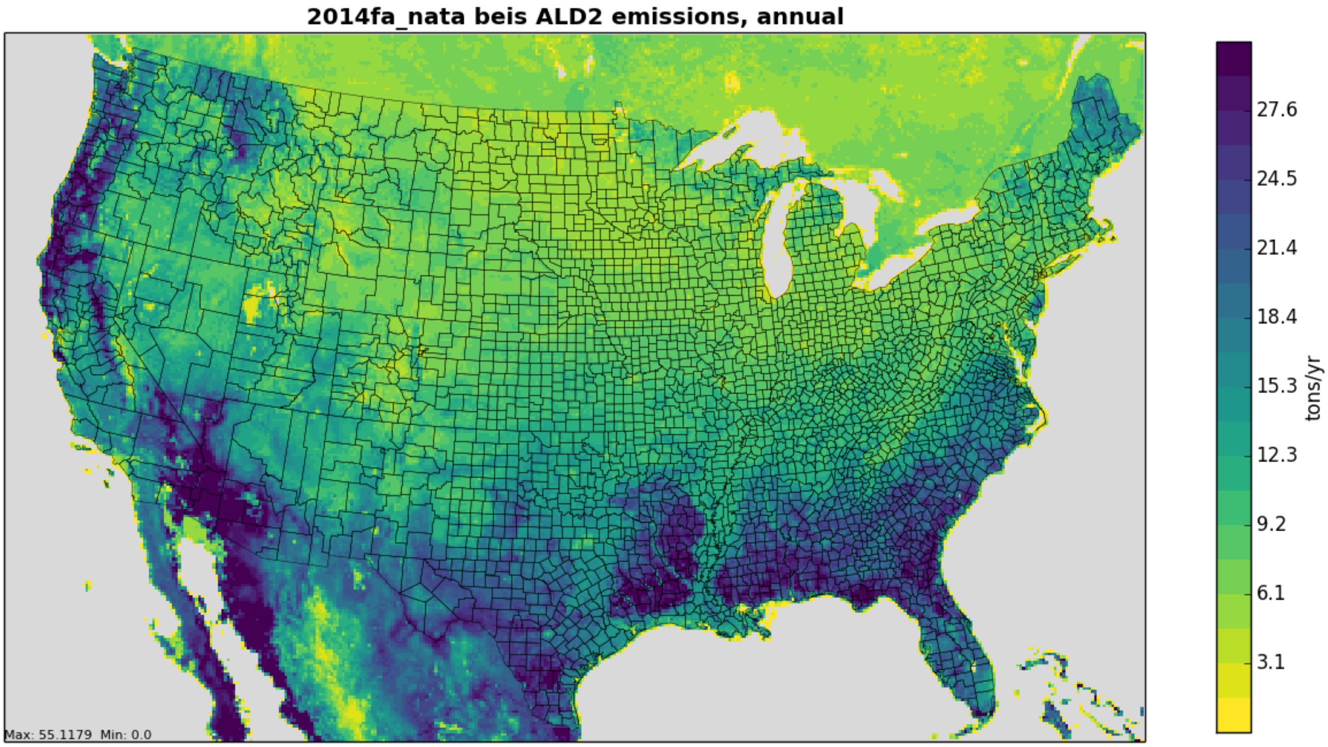
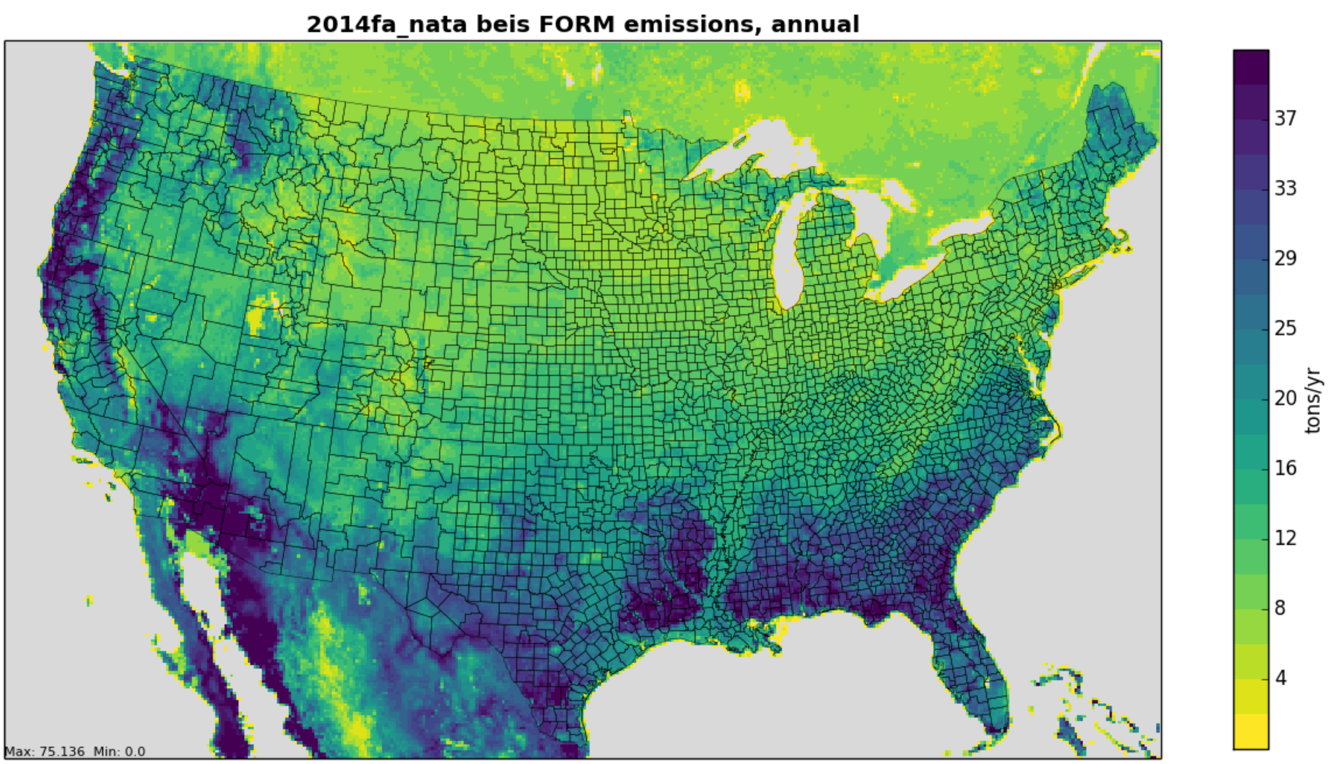


Figure 2-6. Annual formaldehyde emissions output from BEIS 3.61 for 2014



2.8 SMOKE-ready non-anthropogenic inventory for chlorine

The ocean chlorine gas emission estimates are based on the build-up of molecular chlorine (Cl_2) concentrations in oceanic air masses (Bullock and Brehme, 2002). Data at 36 km and 12 km resolution were available and were not modified other than the model-species name “CHLORINE” was changed to “CL2” to support CMAQ modeling.

3 Emissions Modeling Summary

The CMAQ model requires hourly emissions of specific gas and particle species for the horizontal and vertical grid cells contained within the modeled region (i.e., modeling domain). To provide emissions in the form and format required by the model, it is necessary to "pre-process" the "raw" emissions (i.e., emissions input to SMOKE) for the sectors described above in Section 2. In brief, the process of emissions modeling transforms the emissions inventories from their original temporal resolution, pollutant resolution, and spatial resolution into the hourly, speciated, gridded resolution required by the air quality model. Emissions modeling includes temporal allocation, spatial allocation, and pollutant speciation. In some cases, emissions modeling also includes the vertical allocation of point sources, but many air quality models also perform this task because it greatly reduces the size of the input emissions files if the vertical layers of the sources are not included.

As seen in Section 2, the temporal resolutions of the emissions inventories input to SMOKE vary across sectors and may be hourly, daily, monthly, or annual total emissions. The spatial resolution may be individual point sources, county/province/municipio totals, or gridded emissions and varies by sector. This section provides some basic information about the tools and data files used for emissions modeling as part of the modeling platform. In Section 2, the emissions inventories and how they differ from the the previous platform are described. In Section 3, the descriptions of data are limited to the ancillary data SMOKE uses to perform the emissions modeling steps. Note that all SMOKE inputs for the 2015 platform are available from the Air Emissions Modeling website (https://www.epa.gov/air-emissions-modeling/2015-alpha-platform).

SMOKE version 4.5 was used to process the emissions inventories into emissions inputs for each modeling sector into a format compatible with CMAQ. For sectors that have plume rise, the in-line plume rise capability allows for the use of emissions files that are much smaller than full three-dimensional gridded emissions files. For QA of the emissions modeling steps, emissions totals by specie for the entire model domain are output as reports that are then compared to reports generated by SMOKE on the input inventories to ensure that mass is not lost or gained during the emissions modeling process.

3.1 Emissions modeling Overview

When preparing emissions for the air quality model, emissions for each sector are processed separately through SMOKE, and then the final merge program (Mrggrid) is run to combine the model-ready, sector-specific 2-D gridded emissions across sectors. The SMOKE settings in the run scripts and the data in the SMOKE ancillary files control the approaches used by the individual SMOKE programs for each sector. Table 3-1 summarizes the major processing steps of each platform sector. The "Spatial" column shows the spatial approach used: "point" indicates that SMOKE maps the source from a point location (i.e., latitude and longitude) to a grid cell; "surrogates" indicates that some or all of the sources use spatial surrogates to allocate county emissions to grid cells; and "area-to-point" indicates that some of the sources use the SMOKE area-to-point feature to grid the emissions (further described in Section 3.4.2). The "Speciation" column indicates that all sectors use the SMOKE speciation step, though biogenics speciation is done within the Tmpbeis3 program and not as a separate SMOKE step. The "Inventory resolution" column shows the inventory temporal resolution from which SMOKE needs to calculate hourly emissions. Note that for some sectors (e.g., onroad, beis), there is no input inventory; instead, activity data and emission factors are used in combination with meteorological data to compute hourly emissions.

Finally, the "plume rise" column indicates the sectors for which the "in-line" approach is used. These sectors are the only ones with emissions in aloft layers based on plume rise. The term "in-line" means that the plume rise calculations are done inside of the air quality model instead of being computed by SMOKE. The air quality model computes the plume rise using stack parameters and the hourly emissions in the SMOKE output files for each emissions sector. The height of the plume rise determines the model layer into which the emissions are placed. The othpt sector has only "in-line" emissions, meaning that all of the emissions are treated as elevated sources and there are no emissions for those sectors in the two-dimensional, layer-1 files created by SMOKE. Other inline-only sectors are: cmv_c3, ptegu, ptfire, ptfire_othna, ptagfire. Day-specific point fire emissions are treated differently in CMAQ. After plume rise is applied, there are emissions in every layer from the ground up to the top of the plume.

Table 3-1. Key emissions modeling steps by sector.

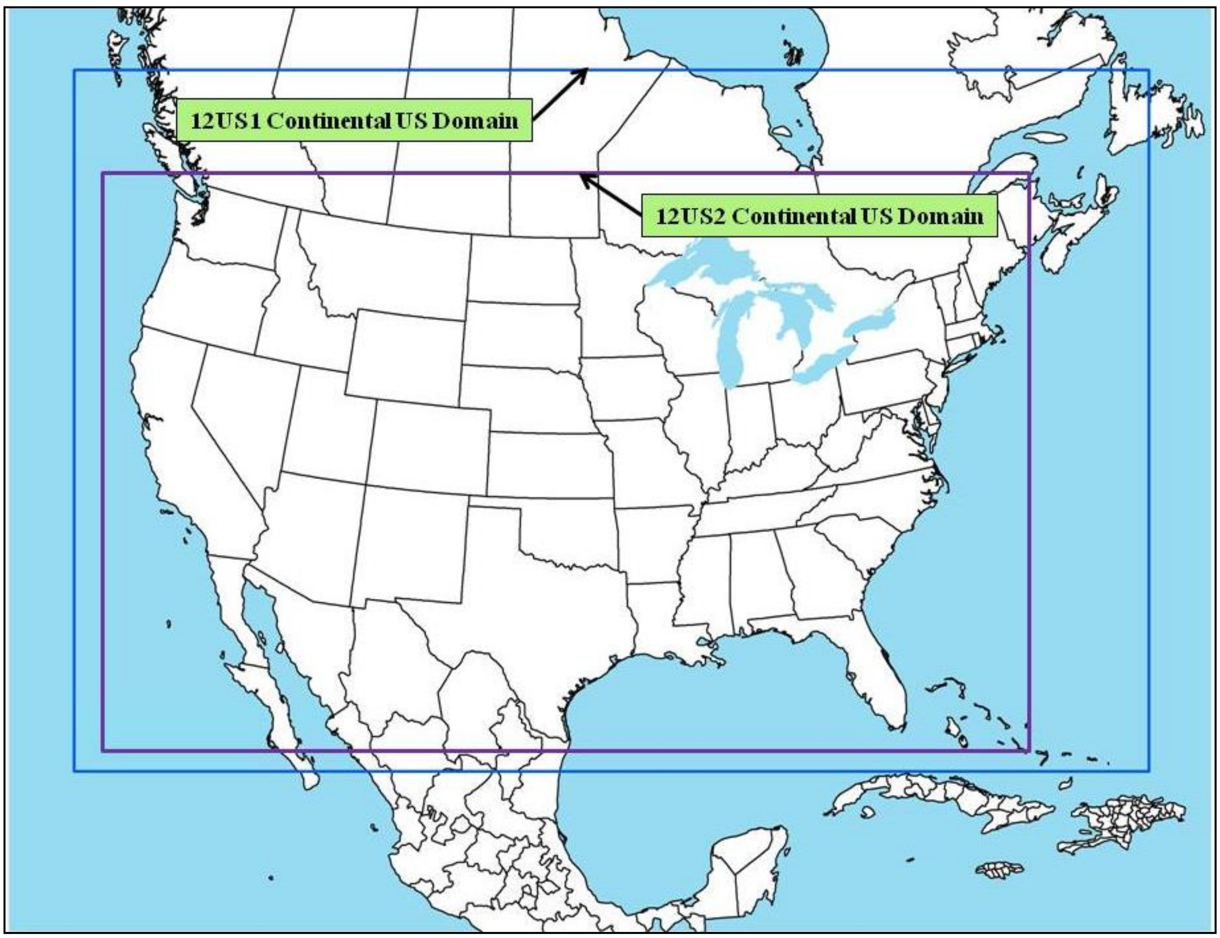
Platform sector	Spatial	Speciation	Inventory resolution	Plume rise
afdust_adj	Surrogates	Yes	annual	
ag	Surrogates	Yes	monthly	
beis	Pre-gridded land use	in BEIS3.61	computed hourly	
cmv_c1c2	Surrogates	Yes	annual	
cmv_c3	Point	Yes	annual	in-line
nonpt	Surrogates & area-to-point	Yes	annual	
nonroad	Surrogates & area-to-point	Yes	monthly	
np_oilgas	Surrogates	Yes	annual	
onroad	Surrogates	Yes	monthly activity, computed hourly	
onroad_ca_adj	Surrogates	Yes	monthly activity, computed hourly	
onroad_can	Surrogates	Yes	monthly	
onroad_mex	Surrogates	Yes	monthly	
othafdust	Surrogates	Yes	annual	
othar	Surrogates	Yes	annual & monthly	
othpt	Point	Yes	annual & monthly	in-line
ptagfire	Point	Yes	daily	in-line
pt_oilgas	Point	Yes	annual	in-line
ptegu	Point	Yes	daily & hourly	in-line
ptfire	Point	Yes	daily	in-line
ptfire_othna	Point	Yes	daily	in-line
ptnonipm	Point	Yes	annual	in-line
rail	Surrogates	Yes	annual	
rwc	Surrogates	Yes	annual	

Biogenic emissions can be modeled two different ways in the CMAQ model. The BEIS model in SMOKE can produce gridded biogenic emissions that are then included in the gridded CMAQ-ready emissions inputs, or alternatively, CMAQ can be configured to create "in-line" biogenic emissions within CMAQ itself. For this platform, biogenic emissions were processed in SMOKE and included in the gridded CMAQ-ready emissions.

SMOKE has the option of grouping sources so that they are treated as a single stack when computing plume rise. For this platform, no grouping was performed because grouping combined with "in-line" processing will not give identical results as "offline" processing (i.e., when SMOKE creates 3-dimensional files). This occurs when stacks with different stack parameters or latitudes/longitudes are grouped, thereby changing the parameters of one or more sources. The most straightforward way to get the same results between in-line and offline is to avoid the use of grouping.

SMOKE was run for the 12US1 modeling domain shown in Figure 3-1 and then the emissions were extracted for the 12US2 domain prior to running the air quality model for this study. Section 3.4 provides the details on the spatial surrogates and area-to-point data used to accomplish spatial allocation with SMOKE.

Figure 3-1. Air quality modeling domains



All grids use a Lambert-Conformal projection, with Alpha = 33º, Beta = 45º and Gamma = -97º, with a center of X = -97º and Y = 40º. Table 3-2 describes the grids for the three domains.

Table 3-2. Descriptions of the platform grids

Common Name	Grid Cell Size	Description (see Figure 3-1)	Grid name	Parameters listed in SMOKE grid description (GRIDDESC) file: projection name, xorig, yorig, xcell, ycell, ncols, nrows, nthik
Continental 12km grid	12 km	Entire conterminous US plus some of Mexico/Canada	12US1_459X299	'LAM_40N97W', -2556000, -1728000, 12.D3, 12.D3, 459, 299, 1
US 12 km or "smaller" CONUS-12	12 km	Smaller 12km CONUS plus some of Mexico/Canada	12US2	'LAM_40N97W', -2412000 , -1620000, 12.D3, 12.D3, 396, 246, 1

3.2 Chemical Speciation

The emissions modeling step for chemical speciation creates the "model species" needed by the air quality model for a specific chemical mechanism. These model species are either individual chemical compounds (i.e., "explicit species") or groups of species (i.e., "lumped species"). The chemical mechanism used for the platform is the CB6 mechanism (Yarwood, 2010). We used a particular version of CB6 that we refer to as "CMAQ CB6" that breaks out naphthalene from XYL as an explicit model species, resulting in model species NAPH and XYLMN instead of XYL and uses SOAALK. This platform generates the $PM_{2.5}$ model species associated with the CMAQ Aerosol Module version 6 (AE6). Table 3-3 lists the model species produced by SMOKE in the platform used for this study. The CB6 mechanism is an update of the older CB05 mechanism. Updates to species assignments for CB05 and CB6 were made for the 2014v7.1 platform and are described in Appendix C.

Table 3-3. Emission model species produced for CB6 for CMAQ

Inventory Pollutant	Model Species	Model species description
Cl_2	CL2	Atomic gas-phase chlorine
HCl	HCL	Hydrogen Chloride (hydrochloric acid) gas
CO	CO	Carbon monoxide
NO_X	NO	Nitrogen oxide
	NO2	Nitrogen dioxide
	HONO	Nitrous acid
SO_2	SO2	Sulfur dioxide
	SULF	Sulfuric acid vapor
NH_3	NH3	Ammonia
	NH3_FERT	Ammonia from fertilizer
VOC	ACET	Acetone
	ALD2	Acetaldehyde
	ALDX	Propionaldehyde and higher aldehydes
	BENZ	Benzene (not part of CB05)
	CH4	Methane
	ETH	Ethene
	ETHA	Ethane
	ETHY	Ethyne
	ETOH	Ethanol
	FORM	Formaldehyde
	IOLE	Internal olefin carbon bond (R-C=C-R)
	ISOP	Isoprene

Inventory Pollutant	Model Species	Model species description
	KET	Ketone Groups
	MEOH	Methanol
	NAPH	Naphthalene
	NVOL	Non-volatile compounds
	OLE	Terminal olefin carbon bond (R-C=C)
	PAR	Paraffin carbon bond
	PRPA	Propane
	SESQ	Sequiterpenes (from biogenics only)
	SOAALK	Secondary Organic Aerosol (SOA) tracer
	TERP	Terpenes (from biogenics only)
	TOL	Toluene and other monoalkyl aromatics
	UNR	Unreactive
	XYLMN	Xylene and other polyalkyl aromatics, minus naphthalene
Naphthalene	NAPH	Naphthalene from inventory
Benzene	BENZ	Benzene from the inventory
Acetaldehyde	ALD2	Acetaldehyde from inventory
Formaldehyde	FORM	Formaldehyde from inventory
Methanol	MEOH	Methanol from inventory
PM_{10}	PMC	Coarse PM > 2.5 microns and ≤ 10 microns
$PM_{2.5}$	PEC	Particulate elemental carbon ≤ 2.5 microns
	PNO3	Particulate nitrate ≤ 2.5 microns
	POC	Particulate organic carbon (carbon only) ≤ 2.5 microns
	PSO4	Particulate Sulfate ≤ 2.5 microns
	PAL	Aluminum
	PCA	Calcium
	PCL	Chloride
	PFE	Iron
	PK	Potassium
	PH2O	Water
	PMG	Magnesium
	PMN	Manganese
	PMOTHR	$PM_{2.5}$ not in other AE6 species
	PNA	Sodium
	PNCOM	Non-carbon organic matter
	PNH4	Ammonium
	PSI	Silica
	PTI	Titanium
Sea-salt species (non – anthropogenic) [6]	PCL	Particulate chloride
	PNA	Particulate sodium

The TOG and $PM_{2.5}$ speciation factors that are the basis of the chemical speciation approach were developed from the SPECIATE 4.5 database (https://www.epa.gov/air-emissions-modeling/speciate), which is the EPA's repository of TOG and PM speciation profiles of air pollution sources. The SPECIATE database development and maintenance is a collaboration involving the EPA's Office of

[6] These emissions are created outside of SMOKE

Research and Development (ORD), Office of Transportation and Air Quality (OTAQ), and the Office of Air Quality Planning and Standards (OAQPS), in cooperation with Environment Canada (EPA, 2016). The SPECIATE database contains speciation profiles for TOG, speciated into individual chemical compounds, VOC-to-TOG conversion factors associated with the TOG profiles, and speciation profiles for $PM_{2.5}$.

Some key features and updates to speciation from previous platforms include the following (the subsections below contain more details on the specific changes):

- VOC speciation profile cross reference assignments for point and nonpoint oil and gas sources were updated to (1) make corrections to the 2011v6.3 cross references, (2) use new and revised profiles that were added to SPECIATE4.5 and (3) account for the portion of VOC estimated to come from flares, based on data from the Oil and Gas estimation tool used to estimate emissions for the NEI. The new/revised profiles included oil and gas operations in specific regions of the country and a national profile for natural gas flares;
- the Western Regional Air Partnership (WRAP) speciation profiles used for the np_oilgas sector are the SPECIATE4.5 revised versions (profiles with "_R" in the profile code);
- the VOC speciation process for nonroad mobile has been updated - profiles are now assigned within MOVES2014a which outputs the emissions with those assignments; also the nonroad profiles themselves were updated;
- VOC and PM speciation for onroad mobile sources occurs within MOVES2014a except for brake and tirewear PM speciation which occurs in SMOKE;
- speciation for onroad mobile sources in Mexico is done within MOVES and is more consistent with that used in the United States;
- the PM speciation profile for C3 ships in the US and Canada was updated to a new profile, 5675AE6; and
- As with previous platforms, some Canadian point source inventories are provided from Environment Canada as pre-speciated emissions; however for the 2013 and 2025 inventories, not all CB6-CMAQ species were provided; missing species were supplemented by speciating VOC which was provided separately.

Speciation profiles and cross-references for this study platform are available in the SMOKE input files for the 2015 platform. Emissions of VOC and $PM_{2.5}$ emissions by county, sector and profile for all sectors other than onroad mobile can be found in the sector summaries for the case.

3.2.1 VOC speciation

The speciation of VOC includes HAP emissions from the 2014NEIv2 in the speciation process. Instead of speciating VOC to generate all of the species listed in Table 3-3, emissions of five specific HAPs: naphthalene, benzene, acetaldehyde, formaldehyde and methanol (collectively known as "NBAFM") from the NEI were "integrated" with the NEI VOC. The integration combines these HAPs with the VOC in a way that does not double count emissions and uses the HAP inventory directly in the speciation process. The basic process is to subtract the specified HAPs emissions mass from the VOC emissions mass, and to then use a special "integrated" profile to speciate the remainder of VOC to the model species excluding the specific HAPs. The EPA believes that the HAP emissions in the NEI are often more representative of emissions than HAP emissions generated via VOC speciation, although this varies by sector.

The NBAFM HAPs were chosen for integration because they are the only explicit VOC HAPs in the CMAQ version 5.2. Explicit means that they are not lumped chemical groups like PAR, IOLE and several other CB6 model species. These "explicit VOC HAPs" are model species that participate in the modeled chemistry using the CB6 chemical mechanism. The use of inventory HAP emissions along with VOC is called "HAP-CAP integration."

The integration of HAP VOC with VOC is a feature available in SMOKE for all inventory formats, including PTDAY (the format used for the ptfire and ptagfire sectors). The ability to use integration with the PTDAY format was made available in the version of SMOKE used for the 2014v7.1 platform, but this new feature is not used for this platform because the ptfire and ptagfire inventories for 2015 do not include HAPs. SMOKE allows the user to specify the particular HAPs to integrate via the INVTABLE. This is done by setting the "VOC or TOG component" field to "V" for all HAP pollutants chosen for integration. SMOKE allows the user to also choose the particular sources to integrate via the NHAPEXCLUDE file (which actually provides the sources to be *excluded* from integration[7]). For the "integrated" sources, SMOKE subtracts the "integrated" HAPs from the VOC (at the source level) to compute emissions for the new pollutant "NONHAPVOC." The user provides NONHAPVOC-to-NONHAPTOG factors and NONHAPTOG speciation profiles[8]. SMOKE computes NONHAPTOG and then applies the speciation profiles to allocate the NONHAPTOG to the other air quality model VOC species not including the integrated HAPs. After determining if a sector is to be integrated, if all sources have the appropriate HAP emissions, then the sector is considered fully integrated and does not need a NHAPEXCLUDE file. If, on the other hand, certain sources do not have the necessary HAPs, then an NHAPEXCLUDE file must be provided based on the evaluation of each source's pollutant mix. The EPA considered CAP-HAP integration for all sectors in determining whether sectors would have full, no or partial integration (see Figure 3-2. Process of integrating NBAFM with VOC for use in VOC Speciation). For sectors with partial integration, all sources are integrated other than those that have either the sum of NBAFM > VOC or the sum of NBAFM = 0.

In this platform, we create NBAFM species from the no-integrate source VOC emissions using speciation profiles. Figure 3-2. Process of integrating NBAFM with VOC for use in VOC Speciation illustrates the integrate and no-integrate processes for U.S. Sources. Since Canada and Mexico inventories do not contain HAPs, we use the approach of generating the HAPs via speciation, except for Mexico onroad mobile sources where emissions for integrate HAPs were available.

It should be noted that even though NBAFM were removed from the SPECIATE profiles used to create the GSPRO for both the NONHAPTOG and no-integrate TOG profiles, there still may be small fractions for "BENZ", "FORM", "ALD2", and "MEOH" present. This is because these model species may have come from species in SPECIATE that are mixtures. The quantity of these model species is expected to be very small compared to the BAFM in the NEI. There are no NONHAPTOG profiles that produce "NAPH."

In SMOKE, the INVTABLE allows the user to specify the particular HAPs to integrate. Two different INVTABLE files are used for different sectors of the platform. For sectors that had no integration across the entire sector (see Table 3-4), EPA created a "no HAP use" INVTABLE in which the "KEEP" flag is

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[7] Since SMOKE version 3.7, the options to specify sources for integration are expanded so that a user can specify the particular sources to include or exclude from integration, and there are settings to include or exclude all sources within a sector. In addition, the error checking is significantly stricter for integrated sources. If a source is supposed to be integrated, but it is missing NBAFM or VOC, SMOKE will now raise an error.

[8] These ratios and profiles are typically generated from the Speciation Tool when it is run with integration of a specified list of pollutants, for example NBAFM.

set to "N" for NBAFM pollutants. Thus, any NBAFM pollutants in the inventory input into SMOKE are automatically dropped. This approach both avoids double-counting of these species and assumes that the VOC speciation is the best available approach for these species for sectors using this approach. The second INVTABLE, used for sectors in which one or more sources are integrated, causes SMOKE to keep the inventory NBAFM pollutants and indicates that they are to be integrated with VOC. This is done by setting the "VOC or TOG component" field to "V" for all five HAP pollutants. Note for the onroad sector, "full integration" includes the integration of benzene, 1,3 butadiene, formaldehyde, acetaldehyde, naphthalene, acrolein, ethyl benzene, 2,2,4-Trimethylpentane, hexane, propionaldehyde, styrene, toluene, xylene, and MTBE.

Figure 3-2. Process of integrating NBAFM with VOC for use in VOC Speciation

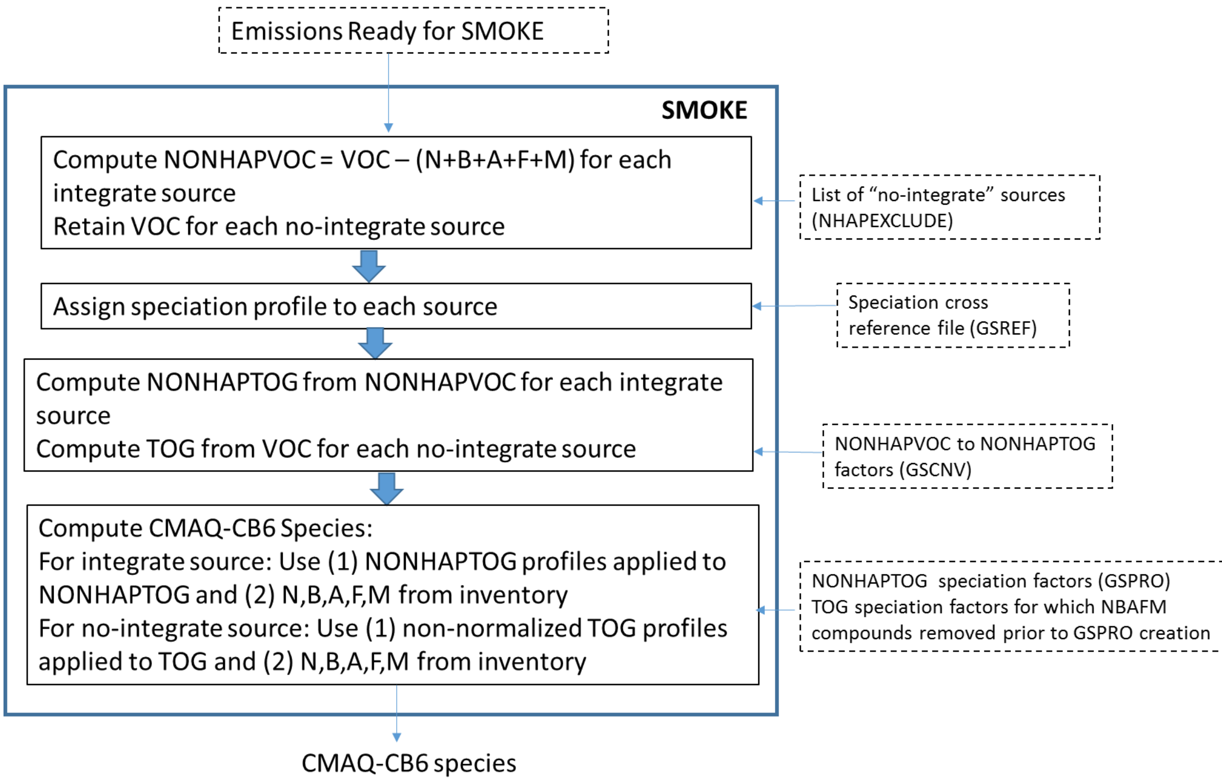


Table 3-4. Integration status of naphthalene, benzene, acetaldehyde, formaldehyde and methanol (NBAFM) for each platform sector

Platform Sector	Approach for Integrating NEI emissions of Naphthalene (N), Benzene (B), Acetaldehyde (A), Formaldehyde (F) and Methanol (M)
ptegu	No integration, create NBAFM from VOC speciation
ptnonipm	No integration, create NBAFM from VOC speciation
ptfire	No integration, no NBAFM in inventory, create NBAFM from VOC speciation
ptfire_othna	No integration, no NBAFM in inventory, create NBAFM from VOC speciation
ptagfire	No integration, no NBAFM in inventory, create NBAFM from VOC speciation
ag	Partial integration (NBAFM)
afdust	N/A – sector contains no VOC
beis	N/A – sector contains no inventory pollutant "VOC"; but rather specific VOC species
cmv_c1c2	Full integration (NBAFM)

Platform Sector	Approach for Integrating NEI emissions of Naphthalene (N), Benzene (B), Acetaldehyde (A), Formaldehyde (F) and Methanol (M)
cmv_c3	Full integration (NBAFM)
rail	Partial integration (NBAFM)
nonpt	Partial integration (NBAFM)
nonroad	Full integration (NBAFM in California, internal to MOVES elsewhere)
np_oilgas	Partial integration (NBAFM)
othpt	No integration, no NBAFM in inventory, create NBAFM from VOC speciation
pt_oilgas	No integration, create NBAFM from VOC speciation
rwc	Partial integration (NBAFM)
onroad	Full integration (internal to MOVES); however, MOVES2014a speciation was CB6-CAMx, not CB6-CMAQ, so post-SMOKE emissions were converted to CB6-CMAQ
onroad_can	No integration, no NBAFM in inventory, create NBAFM from speciation
onroad_mex	Full integration (internal to MOVES-Mexico); however, MOVES-MEXICO speciation was CB6-CAMx, not CB6-CMAQ, so post-SMOKE emissions were converted to CB6-CMAQ
othafdust	N/A – sector contains no VOC
othar	No integration, no NBAFM in inventory, create NBAFM from VOC speciation

Integration for the mobile sources estimated from MOVES (onroad and nonroad sectors, other than for California) is done differently. Briefly there are three major differences: 1) for these sources integration is done using more than just NBAFM, 2) all sources from the MOVES model are integrated and 3) integration is done fully or partially within MOVES. For onroad mobile, speciation is done fully within MOVES2014a such that the MOVES model outputs emission factors for individual VOC model species along with the HAPs. This requires MOVES to be run for a specific chemical mechanism. MOVES was run for the CB6-CAMx mechanism rather than CB6-CMAQ, so post-SMOKE onroad emissions were converted to CB6-CMAQ. More specifically, the CB6-CAMx mechanism excludes XYLMN, NAPH, and SOAALK. After SMOKE processing, we converted the onroad and onroad_mex emissions to CB6-CMAQ as follows:

- XYLMN = XYL[1]-0.966*NAPHTHALENE[1]
- PAR = PAR[1]-0.00001*NAPHTHALENE[1]
- SOAALK = 0.108*PAR[1]

For nonroad mobile, speciation is partially done within MOVES such that it does not need to be run for a specific chemical mechanism. For nonroad, MOVES outputs emissions of HAPs and NONHAPTOG split by speciation profile. Taking into account that integrated species were subtracted out by MOVES already, the appropriate speciation profiles are then applied in SMOKE to get the VOC model species. HAP integration for nonroad uses the same additional HAPs and ethanol as for onroad.

3.2.1.1 County specific profile combinations

SMOKE can compute speciation profiles from mixtures of other profiles in user-specified proportions via two different methods. The first method, which uses a GSPRO_COMBO file, has been in use since the 2005 platform; the second method (GSPRO with fraction) was used for the first time in the 2014v7.0 platform. The GSPRO_COMBO method uses profile combinations specified in the GSPRO_COMBO ancillary file by pollutant (which can include emissions mode, e.g., EXH__VOC), state and county (i.e., state/county FIPS code) and time period (i.e., month). Different GSPRO_COMBO files can be used by sector, allowing for different combinations to be used for different sectors; but within a sector, different profiles cannot be applied based on SCC. The GSREF file indicates that a specific source uses a combination file with the profile code "COMBO." SMOKE computes the resultant profile using the fraction of each specific profile assigned by county, month and pollutant.

In previous platforms, the GSPRO_COMBO feature was used to speciate nonroad mobile and gasoline-related stationary sources that use fuels with varying ethanol content. In these cases, the speciation profiles require different combinations of gasoline profiles, e.g. E0 and E10 profiles. Since the ethanol content varied spatially (e.g., by state or county), temporally (e.g., by month), and by modeling year (future years have more ethanol), the GSPRO_COMBO feature allowed combinations to be specified at various levels for different years. The GSPRO_COMBO is no longer needed for nonroad sources outside of California because nonroad emissions within MOVES have the speciation profiles built into the results, so there is no need to assign them via the GSREF or GSPRO_COMBO feature. For the 2015 platform, GSPRO_COMBO is still used for nonroad sources in California and for certain gasoline-related stationary sources nationwide. The fractions combining the E0 and E10 profiles are based on year 2010 regional fuels and do not vary by month. GSPRO_COMBO is not needed for inventory years after 2016, because the vast majority of fuel is projected to be E10 in future years.

In Canada and Mexico, only E0 speciation profiles are used, but the GSPRO_COMBO feature is still used for inventories where VOC emissions are not explicitly defined by mode (e.g. exhaust versus evaporative). Here, the GSPRO_COMBO specifies a mix of exhaust and evaporative speciation profiles. This is no longer necessary for Canadian mobile sources, whose inventories now include the mode in the pollutant, or for Mexico onroad sources, where VOC speciation is calculated by the MOVES model. For this platform, the GSPRO_COMBO is still used for Mexican nonroad sources which do not have modes in the inventory.

A new method to combine multiple profiles became available in SMOKE4.5. It allows multiple profiles to be combined by pollutant, state and county (i.e., state/county FIPS code) and SCC. This was used specifically for the oil and gas sectors (pt_oilgas and np_oilgas) because SCCs include both controlled and uncontrolled oil and gas operations which use different profiles.

3.2.1.2 Additional sector specific considerations for integrating HAP emissions from inventories into speciation

The decision to integrate HAPs into the speciation was made on a sector by sector basis. For some sectors, there is no integration and VOC is speciated directly; for some sectors, there is full integration meaning all sources are integrated; and for other sectors, there is partial integration, meaning some sources are not integrated and other sources are integrated. The integrated HAPs are either NBAFM or, in the case of MOVES (onroad, nonroad and MOVES-Mexico), a larger set of HAPs plus ethanol are integrated. Table 3-4 above summarizes the integration method for each platform sector.

For the rail sector, the EPA integrated NBAFM for most sources. Some SCCs had zero BAFM and, therefore, they were not integrated. These were SCCs provided by states for which EPA did not do HAP augmentation (2285002008, 2285002009 and 2285002010) because EPA does not create emissions for these SCCs. The VOC for these sources sum to 272 tons, and most of the mass is in California (189 tons) and Washington state (62 tons).

Speciation for the onroad sector is unique. First, SMOKE-MOVES (see Section 2.3.1) is used to create emissions for these sectors and both the MEPROC and INVTABLE files are involved in controlling which pollutants are processed. Second, the speciation occurs within MOVES itself, not within SMOKE. The advantage of using MOVES to speciate VOC is that during the internal calculation of MOVES, the model has complete information on the characteristics of the fleet and fuels (e.g., model year, ethanol content, process, etc.), thereby allowing it to more accurately make use of specific speciation profiles. This means that MOVES produces emission factor tables that include inventory pollutants (e.g., TOG) and model-ready species (e.g., PAR, OLE, etc)[9]. SMOKE essentially calculates the model-ready species by using the appropriate emission factor without further speciation[10]. Third, MOVES' internal speciation uses full integration of an extended list of HAPs beyond NBAFM (called "M-profiles"). The M-profiles integration is very similar to NBAFM integration explained above except that the integration calculation (see Figure 3-2. Process of integrating NBAFM with VOC for use in VOC Speciation) is performed on emissions factors instead of on emissions, and a much larger set of pollutants are integrated besides NBAFM. The list of integrated pollutants is described in Table 3-5. An additional run of the Speciation Tool was necessary to create the M-profiles that were then loaded into the MOVES default database. Fourth, for California, the EPA applied adjustment factors to SMOKE-MOVES to produce California adjusted model-ready files (see Section 2.3.1 for details). By applying the ratios through SMOKE-MOVES, the CARB inventories are essentially speciated to match EPA estimated speciation. This resulted in changes to the VOC HAPs from what CARB submitted to the EPA. Finally, MOVES speciation used the CAMx version of CB6 which does not split out naphthalene.

Table 3-5. MOVES integrated species in M-profiles

MOVES ID	Pollutant Name
5	Methane (CH_4)
20	Benzene
21	Ethanol
22	MTBE
24	1,3-Butadiene
25	Formaldehyde
26	Acetaldehyde
27	Acrolein
40	2,2,4-Trimethylpentane
41	Ethyl Benzene
42	Hexane
43	Propionaldehyde
44	Styrene
45	Toluene
46	Xylene
185	Naphthalene gas

For the nonroad sector, all sources are integrated using the same list of integrated pollutants as shown in Table 3-5. Outside of California, the integration calculations are performed within MOVES. For California, integration calculations are handled by SMOKE. The CARB-based nonroad inventory includes VOC HAP estimates for all sources, so every source in California was integrated as well. Some sources in the original CARB inventory had lower VOC emissions compared to sum of all VOC HAPs. For those sources, VOC was augmented to be equal to the VOC HAP sum, ensuring that every source in

[9] Because the EF table has the speciation "baked" into the factors, all counties that are in the county group (i.e., are mapped to that representative county) will have the same speciation.
[10] For more details on the use of model-ready EF, see the SMOKE 3.7 documentation: https://www.cmascenter.org/smoke/documentation/3.7/html/.

California could be integrated. The CARB-based nonroad data includes exhaust and evaporative mode-specific data for VOC, but, does not contain refueling.

MOVES-MEXICO for onroad used the same speciation approach as for the U.S. in that the larger list of species shown in Table 3-5 was used. However, MOVES-MEXICO used CB6-CAMx, not CB6-CMAQ, so post-SMOKE we converted the emissions to CB6-CMAQ as follows:

- XYLMN = XYL[1]-0.966*NAPHTHALENE[1]
- PAR = PAR[1]-0.00001*NAPHTHALENE[1]
- SOAALK = 0.108*PAR[1]

For most sources in the rwc sector, the VOC emissions were greater than or equal to NBAFM, and NBAFM was not zero, so those sources were integrated, although a few specific sources that did not meet these criteria could not be integrated. In all cases, these sources have SCC= 2104008400 (pellet stoves), and NBAFM > VOC, but not by a significant amount. This results from the sum of NBAFM emission factors exceeding the VOC emission factor. In total, the no-integrate rwc sector sources sum to 4.4 tons VOC and 66 tons of NBAFM. Because for the NATA case the NBAFM are used from the inventory, these no-integrate NBAFM emissions were used in the speciation.

For the nonpt sector, sources for which VOC emissions were greater than or equal to NBAFM, and NBAFM was not zero, were integrated. There is a substantial amount of mass in the nonpt sector that is not integrated: 731,000 tons which is about 20% of the VOC in that sector. It is likely that there would be sources in nonpt that are not integrated because the emission source is not expected to have NBAFM. In fact, 390,000 tons of the no-integrate VOC have no NBAFM in the speciation profiles used for these no-integrate sources. Of the portion of no-integrate VOC with NBAFM there is 3900 tons NBAFM in the profiles (that are dropped from the profiles per the procedure in Figure 3-2. Process of integrating NBAFM with VOC for use in VOC Speciation) for these no-integrate sources.

For the biog sector, the speciation profiles used by BEIS are not included in SPECIATE. The 2011 platform uses BEIS3.61, which includes a new species (SESQ) that was mapped to the model species SESQT. The profile code associated with BEIS3.61 for use with CB05 is "B10C5," while the profile for use with CB6 is "B10C6." The main difference between the profiles is the explicit treatment of acetone emissions in B10C6.

3.2.1.3 Oil and gas related speciation profiles

Most of the new VOC profiles from SPECIATE4.5 listed in Appendix B are for the oil and gas sector. A new national flare profile, FLR99, Natural Gas Flare Profile with DRE >98% was developed from a Flare Test study and used in the v7.0 platform. For the oil and gas sources in the np_oilgas and pt_oilgas sectors, several counties were assigned to newly available basin or area-specific profiles in SPECIATE4.5 that account for measured or modeled from measured compositions specific a particular region of the country. In the 2011 platform, the only county-specific profiles were for the WRAP, but in the 2014 and 2015 platforms, several new profiles were added for other parts of the country. In addition, some of the WRAP profiles were revised to correct for errors such as mole fractions being used for mass fractions and VOCtoTOG factors or replaced with newer data. All WRAP profile codes were renamed to include an "_R" to distinguish between the previous set of profiles (even those that did not change). For the Uintah basin and Denver-Julesburg Basin, Colorado, more updated profiles were used instead of the WRAP Phase III profiles. Table 3-6 lists the region-specific profiles assigned to particular counties or groups of counties. Although this platform increases the use of regional profiles, many counties still rely on the national profiles.

In addition to region-specific assignments, multiple profiles were assigned to particular county/SCC combinations using the SMOKE feature discussed in 3.2.1.1. The profile fractions were computed from VOC emissions provided in an intermediate file generated by the 2014 Nonpoint Oil and Gas Emission Estimation Tool and were updated for the version of the Tool used for the 2014NEIv2. The intermediate file provides flare, non-flare (process), and reboiler (for dehydrators) emissions for six source categories that have flare emissions: Associated Gas, Condensate Tanks, Crude Oil Tanks, Dehydrators, Liquids Unloading and Well Completions by county FIPS and SCC code for the U.S. to account for portions of VOC for a particular VOC that were from controlled emissions or reboiler.

Table 3-6. Basin/Region-specific profiles for oil and gas

Profile Code	Description	Region (if not in the profile name)
DJVNT_R	Denver-Julesburg Basin Produced Gas Composition from Non-CBM Gas Wells	
PNC01_R	Piceance Basin Produced Gas Composition from Non-CBM Gas Wells	
PNC02_R	Piceance Basin Produced Gas Composition from Oil Wells	
PNC03_R	Piceance Basin Flash Gas Composition for Condensate Tank	
PNCDH	Piceance Basin, Glycol Dehydrator	
PRBCB_R	Powder River Basin Produced Gas Composition from CBM Wells	
PRBCO_R	Powder River Basin Produced Gas Composition from Non-CBM Wells	
PRM01_R	Permian Basin Produced Gas Composition for Non-CBM Wells	
SSJCB_R	South San Juan Basin Produced Gas Composition from CBM Wells	
SSJCO_R	South San Juan Basin Produced Gas Composition from Non-CBM Gas Wells	
SWFLA_R	SW Wyoming Basin Flash Gas Composition for Condensate Tanks	
SWVNT_R	SW Wyoming Basin Produced Gas Composition from Non-CBM Wells	
UNT01_R	Uinta Basin Produced Gas Composition from CBM Wells	
WRBCO_R	Wind River Basin Produced Gagres Composition from Non-CBM Gas Wells	
95087a	Oil and Gas - Composite - Oil Field - Oil Tank Battery Vent Gas	East Texas
95109a	Oil and Gas - Composite - Oil Field - Condensate Tank Battery Vent Gas	East Texas
95417	Uinta Basin, Untreated Natural Gas	
95418	Uinta Basin, Condensate Tank Natural Gas	
95419	Uinta Basin, Oil Tank Natural Gas	
95420	Uinta Basin, Glycol Dehydrator	
95398	Composite Profile - Oil and Natural Gas Production - Condensate Tanks	Denver-Julesburg Basin
95399	Composite Profile - Oil Field - Wells	State of California
95400	Composite Profile - Oil Field - Tanks	State of California
95403	Composite Profile - Gas Wells	San Joaquin Basin

3.2.1.4 Mobile source related VOC speciation profiles

The VOC speciation approach for mobile source and mobile source-related source categories is customized to account for the impact of fuels and engine type and technologies. The impact of fuels also affects the parts of the nonpt and ptnonipm sectors that are related to mobile sources such as portable fuel containers and gasoline distribution.

The VOC speciation profiles for the nonroad sector other than for California are listed in Table 3-7. They include new profiles (i.e., those that begin with "953") for 2-stroke and 4-stroke gasoline engines running on E0 and E10 and compression ignition engines with different technologies developed from recent EPA test programs, which also supported the updated toxics emission factor in MOVES2014a (Reichle, 2015 and EPA, 2015b). California nonroad source profiles are presented in Table 3-8.

Table 3-7. TOG MOVES-SMOKE Speciation for nonroad emissions in MOVES2014a

rofile	Profile Description	Engine Type	Engine Technology	Engine Size	Horse-power category	Fuel	Fuel Sub-type	Emission Process
95327	SI 2-stroke E0	SI 2-stroke	all	All	all	Gasoline	E0	exhaust
95328	SI 2-stroke E10	SI 2-stroke	all	All	all	Gasoline	E10	exhaust
95329	SI 4-stroke E0	SI 4-stroke	all	All	all	Gasoline	E0	exhaust
95330	SI 4-stroke E10	SI 4-stroke	all	All	all	Gasoline	E10	exhaust
95331	CI Pre-Tier 1	CI	Pre-Tier 1	All	all	Diesel	all	exhaust
95332	CI Tier 1	CI	Tier 1	all	all	Diesel	all	exhaust
95333	CI Tier 2	CI	Tier 2 and 3	all	all	Diesel	all	exhaust
95333	CI Tier 2	CI	Tier 4	<56 kW (75 hp)	S	Diesel	all	exhaust
8775	ACES Phase 1 Diesel Onroad	CI Tier 4	Tier 4	>=56 kW (75 hp)	L	Diesel	all	exhaust
8753	E0 Evap	SI	all	all	all	Gasoline	E0	evaporative
8754	E10 Evap	SI	all	all	all	Gasoline	E10	evaporative
8766	E0 evap permeation	SI	all	all	all	Gasoline	E0	permeation
8769	E10 evap permeation	SI	all	all	all	Gasoline	E10	permeation
8869	E0 Headspace	SI	all	all	all	Gasoline	E0	headspace
8870	E10 Headspace	SI	all	all	all	Gasoline	E10	headspace
1001	CNG Exhaust	All	all	all	all	CNG	all	exhaust
8860	LPG exhaust	All	all	all	all	LPG	all	exhaust

Speciation profiles for VOC in the nonroad sector account for the ethanol content of fuels across years. A description of the actual fuel formulations for 2014 can be found in the 2014NEIv2 TSD. For previous platforms, the EPA used "COMBO" profiles to model combinations of profiles for E0 and E10 fuel use, but beginning with 2014v7.0 platform, the appropriate allocation of E0 and E10 fuels is done by MOVES.

Combination profiles reflecting a combination of E10 and E0 fuel use are still used for sources upstream of mobile sources such as portable fuel containers (PFCs) and other fuel distribution operations associated with the transfer of fuel from bulk terminals to pumps (BTP) which are in the nonpt sector. They are also used for California nonroad sources. For these sources, ethanol may be mixed into the fuels, in which case speciation would change across years. The speciation changes from fuels in the ptnonipm sector include BTP distribution operations inventoried as point sources. Refinery-to-bulk terminal (RBT) fuel distribution and bulk plant storage (BPS) speciation does not change across the modeling cases because this is considered upstream from the introduction of ethanol into the fuel. The mapping of fuel distribution SCCs to PFC, BTP, BPS, and RBT emissions categories can be found in Appendix F of the 2014v7.1 TSD.

Table 3-8 summarizes the different profiles utilized for the fuel-related sources in each of the sectors. The term "COMBO" indicates that a combination of the profiles listed was used to speciate that subcategory using the GSPRO_COMBO file.

Table 3-8. Select mobile-related VOC profiles

Sector	Sub-category	This platform	
Nonroad- California & non US	gasoline exhaust	COMBO	
		8750a	Pre-Tier 2 E0 exhaust
		8751a	Pre-Tier 2 E10 exhaust
Nonroad-California	gasoline evaporative	COMBO	
		8753	E0 evap
		8754	E10 evap
Nonroad-California	gasoline refueling	COMBO	
		8869	E0 Headspace
		8870	E10 Headspace
Nonroad-California	diesel exhaust	8774	Pre-2007 MY HDD exhaust
Nonroad-California	diesel evaporative and diesel refueling	4547	Diesel Headspace
nonpt/ ptnonipm	PFC and BTP	COMBO	
		8869	E0 Headspace
		8870	E10 Headspace
nonpt/ ptnonipm	Bulk plant storage (BPS) and refine-to-bulk terminal (RBT) sources	8869	E0 Headspace

The speciation of onroad VOC occurs completely within MOVES. MOVES takes into account fuel type and properties, emission standards as they affect different vehicle types and model years, and specific emission processes. Table 3-9 describes all of the M-profiles available to MOVES depending on the model year range, MOVES process (processID), fuel sub-type (fuelSubTypeID), and regulatory class (regClassID). Table 3-10 through Table 3-12 describe the meaning of these MOVES codes. For a specific representative county and future year, there will be a different mix of these profiles. For example, for HD diesel exhaust, the emissions will use a combination of profiles 8774M and 8775M depending on the proportion of HD vehicles that are pre-2007 model years (MY) in that particular county. As that county is projected farther into the future, the proportion of pre-2007 MY vehicles will decrease. A second example, for gasoline exhaust (not including E-85), the emissions will use a combination of profiles 8756M, 8757M, 8758M, 8750aM, and 8751aM. Each representative county has a different mix of these key properties and, therefore, has a unique combination of the specific M-profiles. More detailed information on how MOVES speciates VOC and the profiles used is provided in the technical document, "Speciation of Total Organic Gas and Particulate Matter Emissions from On-road Vehicles in MOVES2014" (EPA, 2015c).

Table 3-9. Onroad M-profiles

Profile	Profile Description	Model Years	ProcessID	FuelSubTypeID	RegClassID
1001M	CNG Exhaust	1940-2050	1,2,15,16	30	48
4547M	Diesel Headspace	1940-2050	11	20,21,22	0
4547M	Diesel Headspace	1940-2050	12,13,18,19	20,21,22	10,20,30,40,41, 42,46,47,48
8753M	E0 Evap	1940-2050	12,13,19	10	10,20,30,40,41,42, 46,47,48
8754M	E10 Evap	1940-2050	12,13,19	12,13,14	10,20,30,40,41, 42,46,47,48
8756M	Tier 2 E0 Exhaust	2001-2050	1,2,15,16	10	20,30
8757M	Tier 2 E10 Exhaust	2001-2050	1,2,15,16	12,13,14	20,30
8758M	Tier 2 E15 Exhaust	1940-2050	1,2,15,16	15,18	10,20,30,40,41, 42,46,47,48
8766M	E0 evap permeation	1940-2050	11	10	0
8769M	E10 evap permeation	1940-2050	11	12,13,14	0
8770M	E15 evap permeation	1940-2050	11	15,18	0
8774M	Pre-2007 MY HDD exhaust	1940-2006	1,2,15,16,17,90	20, 21, 22	40,41,42,46,47, 48
8774M	Pre-2007 MY HDD exhaust	1940-2050	91[11]	20, 21, 22	46,47
8774M	Pre-2007 MY HDD exhaust	1940-2006	1,2,15,16	20, 21, 22	20,30
8775M	2007+ MY HDD exhaust	2007-2050	1,2,15,16	20, 21, 22	20,30
8775M	2007+ MY HDD exhaust	2007-2050	1,2,15,16,17,90	20, 21, 22	40,41,42,46,47,48
8855M	Tier 2 E85 Exhaust	1940-2050	1,2,15,16	50, 51, 52	10,20,30,40,41, 42,46,47,48
8869M	E0 Headspace	1940-2050	18	10	10,20,30,40,41, 42,46,47,48
8870M	E10 Headspace	1940-2050	18	12,13,14	10,20,30,40,41, 42,46,47,48
8871M	E15 Headspace	1940-2050	18	15,18	10,20,30,40,41, 42,46,47,48
8872M	E15 Evap	1940-2050	12,13,19	15,18	10,20,30,40,41, 42,46,47,48
8934M	E85 Evap	1940-2050	11	50,51,52	0
8934M	E85 Evap	1940-2050	12,13,18,19	50,51,52	10,20,30,40,41, 42,46,47,48
8750aM	Pre-Tier 2 E0 exhaust	1940-2000	1,2,15,16	10	20,30
8750aM	Pre-Tier 2 E0 exhaust	1940-2050	1,2,15,16	10	10,40,41,42,46,47,48
8751aM	Pre-Tier 2 E10 exhaust	1940-2000	1,2,15,16	11,12,13,14	20,30
8751aM	Pre-Tier 2 E10 exhaust	1940-2050	1,2,15,16	11,12,13,14,15, 18[12]	10,40,41,42,46,47,48

[11] 91 is the processed for APUs which, are diesel engines not covered by the 2007 Heavy-Duty Rule, so the older technology applied to all years.
[12] The profile assignments for pre-2001 gasoline vehicles fueled on E15/E20 fuels (subtypes 15 and 18) were corrected for MOVES2014a. This model year range, process, fuelsubtype regclass combinate is already assigned to profile 8758.

Table 3-10. MOVES process IDs

Process ID	Process Name
1	Running Exhaust
2	Start Exhaust
9	Brakewear
10	Tirewear
11	Evap Permeation
12	Evap Fuel Vapor Venting
13	Evap Fuel Leaks
15	Crankcase Running Exhaust
16	Crankcase Start Exhaust
17	Crankcase Extended Idle Exhaust
18	Refueling Displacement Vapor Loss
19	Refueling Spillage Loss
20	Evap Tank Permeation
21	Evap Hose Permeation
22	Evap RecMar Neck Hose Permeation
23	Evap RecMar Supply/Ret Hose Permeation
24	Evap RecMar Vent Hose Permeation
30	Diurnal Fuel Vapor Venting
31	HotSoak Fuel Vapor Venting
32	RunningLoss Fuel Vapor Venting
40	Nonroad
90	Extended Idle Exhaust
91	Auxiliary Power Exhaust

Table 3-11. MOVES Fuel subtype IDs

Fuel Subtype ID	Fuel Subtype Descriptions
10	Conventional Gasoline
11	Reformulated Gasoline (RFG)
12	Gasohol (E10)
13	Gasohol (E8)
14	Gasohol (E5)
15	Gasohol (E15)
18	Ethanol (E20)
20	Conventional Diesel Fuel
21	Biodiesel (BD20)
22	Fischer-Tropsch Diesel (FTD100)
30	Compressed Natural Gas (CNG)
50	Ethanol
51	Ethanol (E85)
52	Ethanol (E70)

Table 3-12. MOVES regclass IDs

Reg. Class ID	Regulatory Class Description
0	Doesn't Matter
10	Motorcycles
20	Light Duty Vehicles
30	Light Duty Trucks
40	Class 2b Trucks with 2 Axles and 4 Tires (8,500 lbs < GVWR <= 10,000 lbs)
41	Class 2b Trucks with 2 Axles and at least 6 Tires or Class 3 Trucks (8,500 lbs < GVWR <= 14,000 lbs)
42	Class 4 and 5 Trucks (14,000 lbs < GVWR <= 19,500 lbs)
46	Class 6 and 7 Trucks (19,500 lbs < GVWR <= 33,000 lbs)
47	Class 8a and 8b Trucks (GVWR > 33,000 lbs)
48	Urban Bus (see CFR Sec 86.091_2)

For portable fuel containers (PFCs) and fuel distribution operations associated with the bulk-plant-to-pump (BTP) distribution, ethanol may be mixed into the fuels; therefore, county- and month-specific COMBO speciation was used (via the GSPRO_COMBO file). Refinery to bulk terminal (RBT) fuel distribution and bulk plant storage (BPS) speciation are considered upstream from the introduction of ethanol into the fuel; therefore, a single profile is sufficient for these sources. No refined information on potential VOC speciation differences between cellulosic diesel and cellulosic ethanol sources was available; therefore, cellulosic diesel and cellulosic ethanol sources used the same SCC (30125010: Industrial Chemical Manufacturing, Ethanol by Fermentation production) for VOC speciation as was used for corn ethanol plants.

3.2.2 PM speciation

In addition to VOC profiles, the SPECIATE database also contains profiles for speciating $PM_{2.5.}$ We speciated $PM_{2.5}$ into the AE6 species associated with CMAQ 5.0.1 and later versions. Most of the PM profiles come from the 911XX series (Reff et. al, 2009), which include updated AE6 speciation[13]. Starting with the 2014v7.1 platform, we replaced profile 91112 (Natural Gas Combustion – Composite) with 95475 (Composite -Refinery Fuel Gas and Natural Gas Combustion). This updated profile is an AE6-ready profile based on the median of 3 SPECIATE4.5 profiles from which AE6 versions were made (to be added to SPECIATE5.0): boilers (95125a), process heaters (95126a) and internal combustion combined cycle/cogen plant exhaust (95127a). As with profile 91112, these profiles are based on tests using natural gas and refinery fuel gas (England et al., 2007). Profile 91112 which is also based on refinery gas and natural gas is thought to overestimate EC.
Profile 95475 (Composite -Refinery Fuel Gas and Natural Gas Combustion) is shown along with the underlying profiles composited in Figure 3-3. Figure 3-4 shows a comparison of the new profile which the one that we had been using in the 2014v7.0 and earlier platforms.

[13] The exceptions are 5675AE6 (Marine Vessel – Marine Engine – Heavy Fuel Oil) used for cmv_c3 and 92018 (Draft Cigarette Smoke – Simplified) used in nonpt. 5675AE6 is an update of profile 5675 to support AE6 PM speciation.

Figure 3-3. Profiles composited for the new PM gas combustion related sources

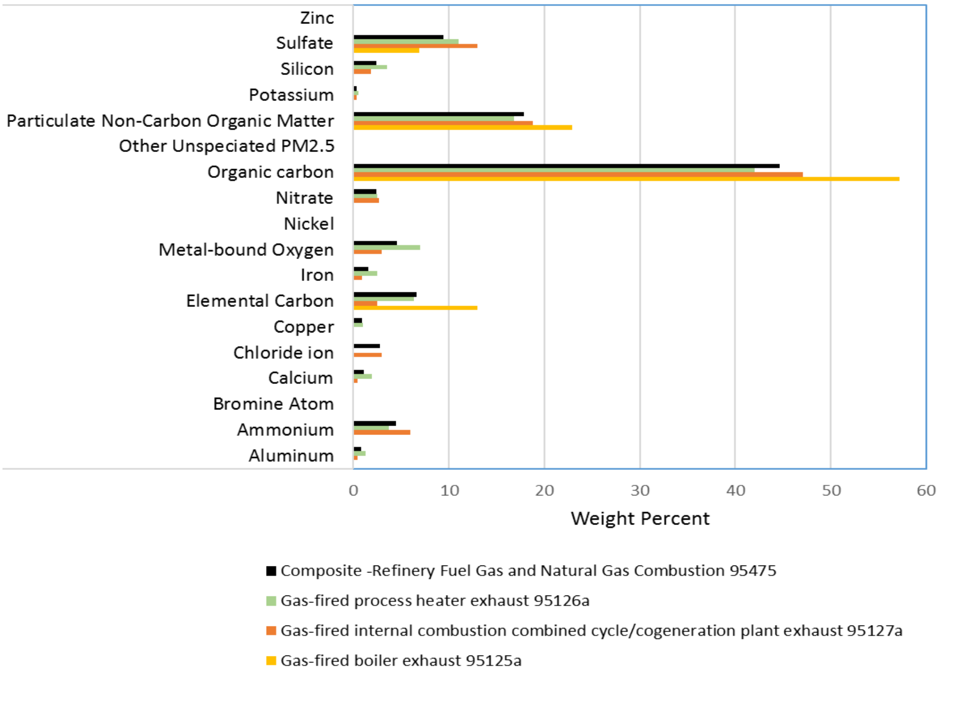
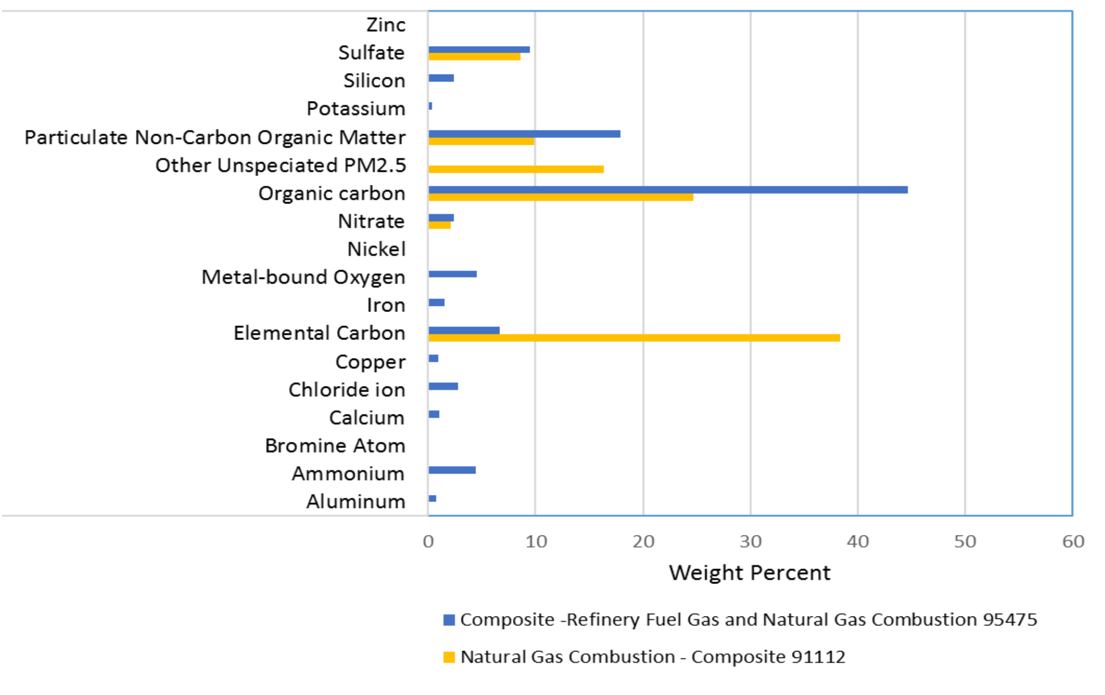


Figure 3-4. Comparison of PM profiles used for Natural gas combustion related sources



3.2.2.1 Mobile source related PM2.5 speciation profiles

For the onroad sector, for all processes except brake and tire wear, PM speciation occurs within MOVES itself, not within SMOKE (similar to the VOC speciation described above). The advantage of using MOVES to speciate PM is that during the internal calculation of MOVES, the model has complete information on the characteristics of the fleet and fuels (e.g., model year, sulfur content, process, etc.) to accurately match to specific profiles. This means that MOVES produces EF tables that include total PM (e.g., PM_{10} and $PM_{2.5}$) and speciated PM (e.g., PEC, PFE, etc). SMOKE essentially calculates the PM components by using the appropriate EF without further speciation[14]. The specific profiles used within MOVES include two compressed natural gas (CNG) profiles, 45219 and 45220, which were added to SPECIATE4.5. A list of profiles is provided in the technical document, "Speciation of Total Organic Gas and Particulate Matter Emissions from On-road Vehicles in MOVES2014" (EPA, 2015c).

For onroad brake and tire wear, the PM is speciated in the *moves2smk* postprocessor that prepares the emission factors for processing in SMOKE. The formulas for this are based on the standard speciation factors from brake and tire wear profiles, which were updated from the v6.3 platform based on data from a Health Effects Institute report (Schauer, 2006). Table 3-13 shows the differences in the v7.1 and v6.3 profiles.

Table 3-13. SPECIATE4.5 brake and tire profiles compared to those used in the 2011v6.3 Platform

Inventory Pollutant	Model Species	V6.3 platform brakewear profile: 91134	SPECIATE4.5 brakewear profile: 95462 from Schauer (2006)	V6.3 platform tirewear profile: 91150	SPECIATE4.5 tirewear profile: 95460 from Schauer (2006)
PM2_5	PAL	0.00124	0.000793208	6.05E-04	3.32401E-05
PM2_5	PCA	0.01	0.001692177	0.00112	
PM2_5	PCL	0.001475		0.0078	
PM2_5	PEC	0.0261	0.012797085	0.22	0.003585907
PM2_5	PFE	0.115	0.213901692	0.0046	0.00024779
PM2_5	PH2O	0.0080232		0.007506	
PM2_5	PK	1.90E-04	0.000687447	3.80E-04	4.33129E-05
PM2_5	PMG	0.1105	0.002961309	3.75E-04	0.000018131
PM2_5	PMN	0.001065	0.001373836	1.00E-04	1.41E-06
PM2_5	PMOTHR	0.4498	0.691704999	0.0625	0.100663209
PM2_5	PNA	1.60E-04	0.002749787	6.10E-04	7.35312E-05
PM2_5	PNCOM	0.0428	0.020115749	0.1886	0.255808124
PM2_5	PNH4	3.00E-05		1.90E-04	
PM2_5	PNO3	0.0016		0.0015	
PM2_5	POC	0.107	0.050289372	0.4715	0.639520309
PM2_5	PSI	0.088		0.00115	
PM2_5	PSO4	0.0334		0.0311	
PM2_5	PTI	0.0036	0.000933341	3.60E-04	5.04E-06

The formulas used based on brake wear profile 95462 and tire wear profile 95460 are as follows:

```
POC = 0.6395 * PM25TIRE + 0.0503 * PM25BRAKE
PEC = 0.0036 * PM25TIRE + 0.0128 * PM25BRAKE
```

[14] Unlike previous platforms, the PM components (e.g., POC) are now consistently defined between MOVES2014 and CMAQ. For more details on the use of model-ready EF, see the SMOKE 3.7 documentation: https://www.cmascenter.org/smoke/documentation/3.7/html/.

```
PNO3 = 0.000 * PM25TIRE + 0.000 * PM25BRAKE
PSO4 = 0.0 * PM25TIRE + 0.0 * PM25BRAKE
PNH4 = 0.000 * PM25TIRE + 0.0000 * PM25BRAKE
PNCOM = 0.2558 * PM25TIRE + 0.0201 * PM25BRAKE
```

For California onroad emissions, adjustment factors were applied to SMOKE-MOVES to produce California adjusted model-ready files (see Section 2.3.1 for details). California did not supply speciated PM, therefore, the adjustment factors applied to PM2.5 were also applied to the speciated PM components. By applying the ratios through SMOKE-MOVES, the CARB inventories are essentially speciated to match EPA estimated speciation.

For nonroad PM2.5, speciation is done in SMOKE similarly to nonpoint and point categories based on the GSREF SCC-to-speciation profile cross reference file. There are only 3 unique PM2.5 profiles assigned to the hundreds of nonroad SCCs.

Table 3-14. Nonroad PM2.5 profiles

SPECIATE4.5 Profile Code	SPECIATE4.5 Profile Name	Assigned to Nonroad sources based on Fuel Type
91106	HDDV Exhaust - Composite	Diesel
91113	Nonroad Gasoline Exhaust - Composite	Gasoline
91156	Residential Natural Gas Combustion - Composite	LPG, CNG

3.2.3 NO_X speciation

NOx emission factors and therefore NOx inventories are developed on a NO_2 weight basis. For air quality modeling, NO_X is speciated into NO, NO_2, and/or HONO. For the non-mobile sources, the EPA used a single profile “NHONO” to split NO_X into NO and NO_2.

The importance of HONO chemistry, identification of its presence in ambient air and the measurements of HONO from mobile sources have prompted the inclusion of HONO in NOx speciation for mobile sources. Based on tunnel studies, a HONO to NOx ratio of 0.008 was chosen (Sarwar, 2008). For the mobile sources, except for onroad (including nonroad, cmv, rail, othon sectors), and for specific SCCs in othar and ptnonipm, the profile “HONO” is used. Table 3-15 gives the split factor for these two profiles. The onroad sector does not use the “HONO” profile to speciate NO_X. MOVES2014 produces speciated NO, NO_2, and HONO by source, including emission factors for these species in the emission factor tables used by SMOKE-MOVES. Within MOVES, the HONO fraction is a constant 0.008 of NO_X. The NO fraction varies by heavy duty versus light duty, fuel type, and model year.
The NO_2 fraction = 1 – NO – HONO. For more details on the NO_X fractions within MOVES, https://nepis.epa.gov/Exe/ZyPDF.cgi?Dockey=P100F1A5.pdf .

Table 3-15. NO_X speciation profiles

Profile	pollutant	species	split factor
HONO	NOX	NO2	0.092
HONO	NOX	NO	0.9
HONO	NOX	HONO	0.008
NHONO	NOX	NO2	0.1
NHONO	NOX	NO	0.9

3.2.4 Creation of Sulfuric Acid Vapor (SULF)

Since at least the 2002 Platform, sulfuric acid vapor (SULF) has been estimated through the SMOKE speciation process for coal combustion and residual and distillate oil fuel combustion sources. Profiles that compute SULF from SO_2 are assigned to coal and oil combustion SCCs in the GSREF ancillary file. The profiles were derived from information from AP-42 (EPA, 1998), which identifies the fractions of sulfur emitted as sulfate and SO_2 and relates the sulfate as a function of SO2.

Sulfate is computed from SO_2 assuming that gaseous sulfate, which is comprised of many components, is primarily H_2SO_4. The equation for calculating H_2SO_4 is given below.

$$Emissions\ of\ SULF\ (as\ \mathrm{H2SO4}) = SO2\ emissions\ \times \frac{fraction\ of\ S\ emitted\ as\ sulfate}{fraction\ of\ S\ emitted\ as\ SO2} \times \frac{MW\ H2SO4}{MW\ SO2}$$

In the above, *MW* is the molecular weight of the compound. The molecular weights of H_2SO_4 and SO_2 are 98 g/mol and 64 g/mol, respectively.

This method does not reduce SO_2 emissions; it solely adds gaseous sulfate emissions as a function of SO2 emissions. The derivation of the profiles is provided in Table 3-16; a summary of the profiles is provided in Table 3-17.

Table 3-16. Sulfate split factor computation

fuel	SCCs	Profile Code	Fraction as SO2	Fraction as sulfate	Split factor (mass fraction)
Bituminous	1-0X-002-YY, where X is 1, 2 or 3 and YY is 01 thru 19 and 21-ZZ-002-000 where ZZ is 02,03 or 04	95014	0.95	0.014	.014/.95 * 98/64 = 0.0226
Subbituminous	1-0X-002-YY, where X is 1, 2 or 3 and YY is 21 thru 38	87514	.875	0.014	.014/.875 * 98/64 = 0.0245
Lignite	1-0X-003-YY, where X is 1, 2 or 3 and YY is 01 thru 18 and 21-ZZ-002-000 where ZZ is 02,03 or 04	75014	0.75	0.014	.014/.75 * 98/64 = 0.0286
Residual oil	1-0X-004-YY, where X is 1, 2 or 3 and YY is 01 thru 06 and 21-ZZ-005-000 where ZZ is 02,03 or 04	99010	0.99	0.01	.01/.99 * 98/64 = 0.0155
Distillate oil	1-0X-005-YY, where X is 1, 2 or 3 and YY is 01 thru 06 and 21-ZZ-004-000 where ZZ is 02,03 or 04	99010	0.99	0.01	Same as residual oil

Table 3-17. SO_2 speciation profiles

Profile	pollutant	species	split factor
95014	SO2	SULF	0.0226
95014	SO2	SO2	1
87514	SO2	SULF	0.0245
87514	SO2	SO2	1
75014	SO2	SULF	0.0286
75014	SO2	SO2	1
99010	SO2	SULF	0.0155
99010	SO2	SO2	1

3.3 Temporal Allocation

Temporal allocation is the process of distributing aggregated emissions to a finer temporal resolution, thereby converting annual emissions to hourly emissions as is required by CMAQ. While the total emissions are important, the timing of the occurrence of emissions is also essential for accurately simulating ozone, PM, and other pollutant concentrations in the atmosphere. Many emissions inventories are annual or monthly in nature. Temporal allocation takes these aggregated emissions and distributes the emissions to the hours of each day. This process is typically done by applying temporal profiles to the inventories in this order: monthly, day of the week, and diurnal, with monthly and day-of-week profiles applied only if the inventory is not already at that level of detail.

The temporal factors applied to the inventory are selected using some combination of country, state, county, SCC, and pollutant. Table 3-18 summarizes the temporal aspects of emissions modeling by comparing the key approaches used for temporal processing across the sectors. In the table, “Daily temporal approach” refers to the temporal approach for getting daily emissions from the inventory using the SMOKE Temporal program. The values given are the values of the SMOKE L_TYPE setting. The "Merge processing approach" refers to the days used to represent other days in the month for the merge step. If this is not "all," then the SMOKE merge step runs only for representative days, which could include holidays as indicated by the right-most column. The values given are those used for the SMOKE M_TYPE setting (see below for more information).

Table 3-18. Temporal settings used for the platform sectors in SMOKE

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	Monthly		met-based	all	No
beis	Hourly		n/a	all	No
cmv_c1c2	Annual	Yes	aveday	aveday	No
cmv_c3	Annual	Yes	aveday	aveday	No
nonpt	Annual	Yes	week	week	Yes
nonroad	Monthly		mwdss	mwdss	Yes
np_oilgas	Annual	Yes	week	week	Yes
onroad	Annual & monthly[1]		all	all	Yes
onroad_ca_adj	Annual & monthly[1]		all	all	Yes
othafdust_adj	Annual	Yes	week	week	No
othar	Annual & monthly	Yes	week	week	No
onroad_can	Monthly		week	week	No
onroad_mex	Monthly		week	week	No
othpt	Annual & monthly	Yes	mwdss	mwdss	No
ptagfire	Daily		all	all	No
pt_oilgas	Annual	Yes	mwdss	mwdss	Yes
ptegu	Annual & hourly	Yes[2]	all	all	No
ptnonipm	Annual	Yes	mwdss	mwdss	Yes
ptfire	Daily		all	all	No
ptfire_othna	Daily		all	all	No
rail	Annual	Yes	aveday	aveday	No
rwc	Annual	No[3]	met-based	all	No[3]

[1]Note the annual and monthly "inventory" actually refers to the activity data (VMT, hoteling and VPOP) for onroad. VMT and hoteling is monthly and VPOP is annual. The actual emissions are computed on an hourly basis.
[2]Only units that do not have matching hourly CEMS data use monthly temporal profiles.
[3]Except for 2 SCCs that do not use met-based temporalization.

The following values are used in the table. The value "all" means that hourly emissions are computed for every day of the year and that emissions potentially have day-of-year variation. The value "week" means that hourly emissions computed for all days in one "representative" week, representing all weeks for each month. This means emissions have day-of-week variation, but not week-to-week variation within the month. The value "mwdss" means hourly emissions for one representative Monday, representative weekday (Tuesday through Friday), representative Saturday, and representative Sunday for each month. This means emissions have variation between Mondays, other weekdays, Saturdays and Sundays within the month, but not week-to-week variation within the month. The value "aveday" means hourly emissions computed for one representative day of each month, meaning emissions for all days within a month are the same. Special situations with respect to temporal allocation are described in the following subsections.

In addition to the resolution, temporal processing includes a ramp-up period for several days prior to January 1, 2016, which is intended to mitigate the effects of initial condition concentrations. The ramp-up period was 10 days (December 22-31, 2015). For most sectors, emissions from December 2016 (representative days) were used to fill in emissions for the end of December 2015. For biogenic emissions, December 2015 emissions were processed using 2015 meteorology.

3.3.1 Use of FF10 format for finer than annual emissions

The FF10 inventory format for SMOKE provides a consolidated format for monthly, daily, and hourly emissions inventories. With the FF10 format, a single inventory file can contain emissions for all 12 months and the annual emissions in a single record. This helps simplify the management of numerous inventories. Similarly, daily and hourly FF10 inventories contain individual records with data for all days in a month and all hours in a day, respectively.

SMOKE prevents the application of temporal profiles on top of the "native" resolution of the inventory. For example, a monthly inventory should not have annual-to-month temporal allocation applied to it; rather, it should only have month-to-day and diurnal temporal allocation. This becomes particularly important when specific sectors have a mix of annual, monthly, daily, and/or hourly inventories. The flags that control temporal allocation for a mixed set of inventories are discussed in the SMOKE documentation. The modeling platform sectors that make use of monthly values in the FF10 files are ag, nonroad, onroad, onroad_can, onroad_mex, othar, and othpt.

3.3.2 Electric Generating Utility temporal allocation (ptegu)

3.3.2.1 Base year temporal allocation of EGUs

The 2015 annual EGU emissions not matched to CEMS sources use region/fuel specific profiles based on average hourly emissions for the region and fuel. Peaking units were removed during the averaging to minimize the spikes generated by those units. The non-matched units are allocated to hourly emissions using the following three-step methodology: annual value to month, month to day, and day to hour. First, the CEMS data were processed using a tool that reviewed the data quality flags that indicate the data were not measured. Unmeasured data can be filled in with maximum values and thereby cause erroneously high values in the CEMS data. The CEMCorrect tool identifies hours for which the data were not measured. When those values are found to be more than three times the annual mean for that unit, the data for those hours are replaced with annual mean values (Adelman et al., 2012). These adjusted CEMS data were then used for the remainder of the temporal allocation process described below (see Figure 3-5 for an example). Winter and summer seasons are included in the development of the diurnal profiles as opposed to using data for the entire year because analysis of the hourly CEMS data revealed that there were different diurnal patterns in winter versus summer in many areas. Typically, a single mid-day peak is visible in the summer, while there are morning and evening peaks in the winter as shown in Figure 3-6.

The temporal allocation procedure is differentiated by whether or not the source could be directly matched to a CEMS unit via ORIS facility code and boiler ID. Note that for units matched to CEMS data, annual totals of their emissions input to CMAQ may be different than the annual values in 2015 because the CEMS data replaces the NO_x and SO_2 inventory data for the seasons in which the CEMS are operating. If a CEMS-matched unit is determined to be a partial year reporter, as can happen for sources that run CEMS only in the summer, emissions totaling the difference between the annual emissions and the total CEMS emissions are allocated to the non-summer months.

Figure 3-5. Eliminating unmeasured spikes in CEMS data

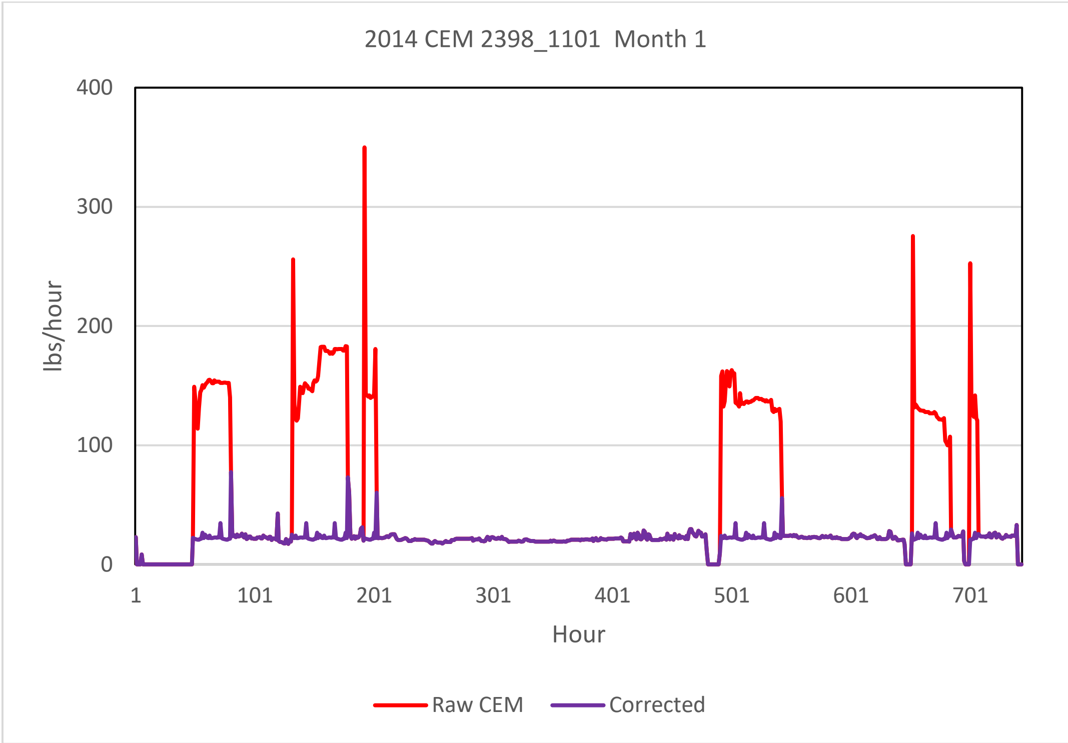
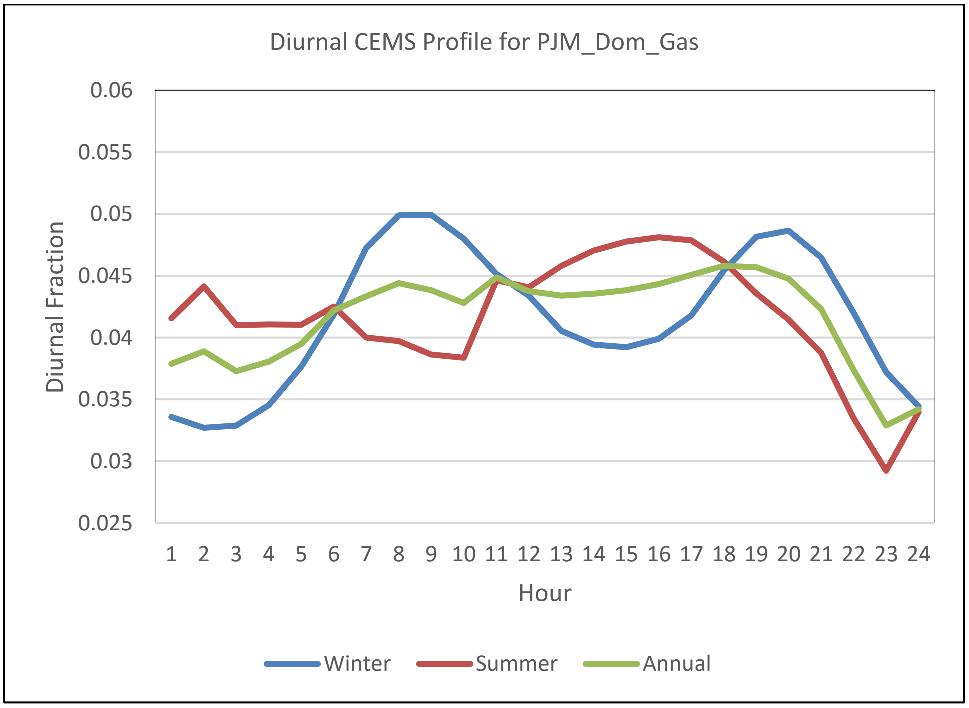


Figure 3-6. Seasonal diurnal profiles for EGU emissions in a Virginia Region



For sources not matched to CEMS units, temporal profiles are calculated that are used by SMOKE to allocate the annual emissions to hourly values. For these units, the allocation of the inventory annual emissions to months is done using average fuel-specific annual-to-month factors generated for each of the 64 IPM regions shown in Figure 3-7. These factors are based on 2015 CEMS data only. In each region, separate factors were developed for the fuels: coal, natural gas, and “other,” where the types of fuels included in “other” vary by region. Separate profiles were computed for NO_X, SO_2, and heat input. An overall composite profile was also computed and used when there were no CEMS units with the specified fuel in the region containing the unit. For both CEMS-matched units and units not matched to CEMS, NO_X and SO_2 CEMS data are used to allocate NO_X and SO_2 emissions to monthly emissions, respectively, while heat input data are used to allocate emissions of all pollutants from monthly to daily emissions.

Daily temporal allocation of units matched to CEMS was performed using a procedure similar to the approach to allocate emissions to months in that the CEMS data replaces the inventory data for each pollutant. For units without CEMS data, emissions were allocated from month to day using IPM-region and fuel-specific average month-to-day factors based on the 2015 CEMS heat input data. Separate month-to-day allocation factors were computed for each month of the year using heat input for the fuels coal, natural gas, and “other” in each region. For CEMS matched units, NO_X and SO_2 CEMS data are used to replace inventory NO_X and SO_2 emissions, while CEMS heat input data are used to allocate all other pollutants. An example of month-to-day profiles for gas, coal, and an overall composite for a region in western Texas is shown in Figure 3-8.

For units matched to CEMS data, hourly emissions use the hourly CEMS values for NO_X and SO_2, while other pollutants are allocated according to heat input values. For units not matched to CEMS data, temporal profiles from days to hours are computed based on the season-, region- and fuel-specific average day-to-hour factors derived from the CEMS data for those fuels and regions using the appropriate subset of data. For the unmatched units, CEMS heat input data are used to allocate all pollutants (including NO_X and SO_2) because the heat input data was generally found to be more complete than the pollutant-specific data. SMOKE then allocates the daily emissions data to hours using the temporal profiles obtained from the CEMS data for the analysis base year (i.e., 2015 in this case).

Certain sources without CEMS data, such as specific municipal waste combustors (MWCs) and cogeneration facilities (cogens), were assigned a flat temporal profile by source. The emissions for these sources have an equal value for each hour of the year.

Figure 3-7. IPM Regions used to Create Temporal Profiles for EGUs without CEMS

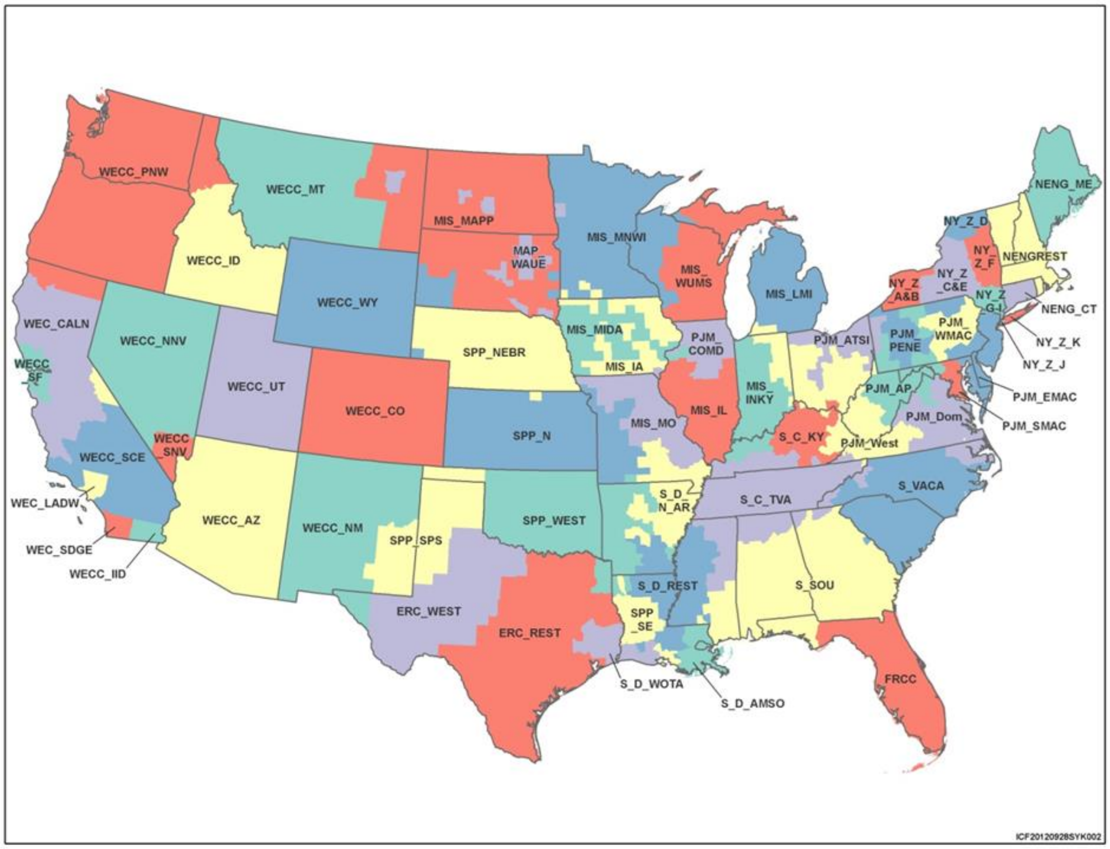
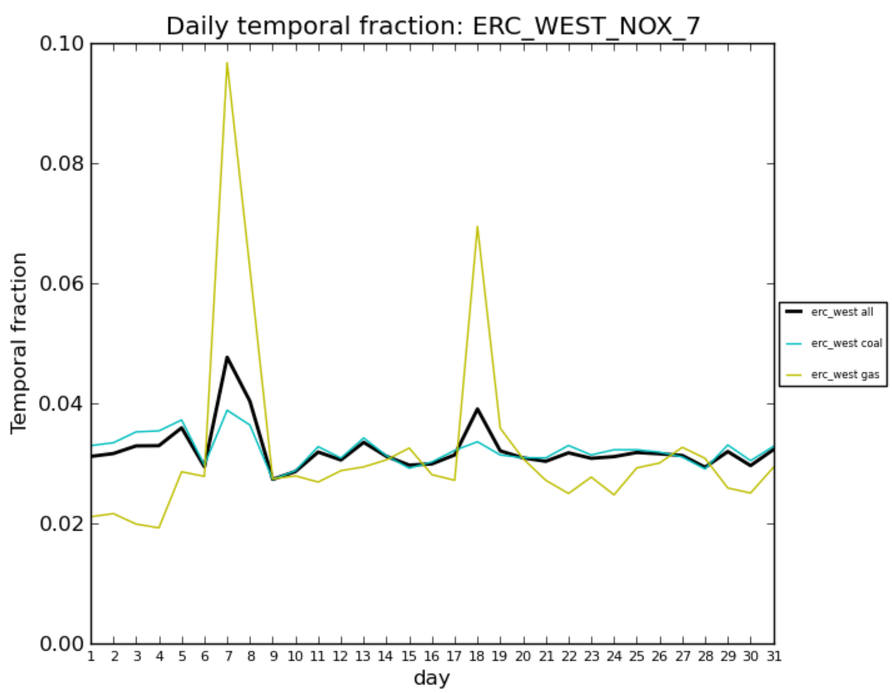


Figure 3-8. Month-to-day profiles for different fuels in a West Texas Region



3.3.3 Airport Temporal allocation (ptnonipm)

Airport temporal profiles were updated in 2014v7.0 and were kept the same for 2014v7.1 and 2015 platform. All airport SCCs (i.e., 2275*, 2265008005, 2267008005, 2268008005 and 2270008005) were given the same hourly, weekly and monthly profile for all airports other than Alaska seaplanes (which are not in the CMAQ modeling domain). Hourly airport operations data were obtained from the Aviation System Performance Metrics (ASPM) Airport Analysis website (https://aspm.faa.gov/apm/sys/AnalysisAP.asp). A report of 2014 hourly Departures and Arrivals for Metric Computation was generated. An overview of the ASPM metrics is at http://aspmhelp.faa.gov/index.php/Aviation_Performance_Metrics_%28APM%29. Figure 3-9 shows the diurnal airport profile.

Weekly and monthly temporal profiles are based on 2014 data from the FAA Operations Network Air Traffic Activity System (http://aspm.faa.gov/opsnet/sys/Terminal.asp). A report of all airport operations (takeoffs and landings) by day for 2014 was generated. These data were then summed to month and day-of-week to derive the monthly and weekly temporal profiles shown in Figure 3-9, Figure 3-10, and Figure 3-11. An overview of the Operations Network data system is at http://aspmhelp.faa.gov/index.php/Operations_Network_%28OPSNET%29.

Alaska seaplanes, which are outside the CONUS domain use the same monthly profile as in the 2011 platform shown in Figure 3-12. These were assigned based on the facility ID.

Figure 3-9. Diurnal Profile for all Airport SCCs

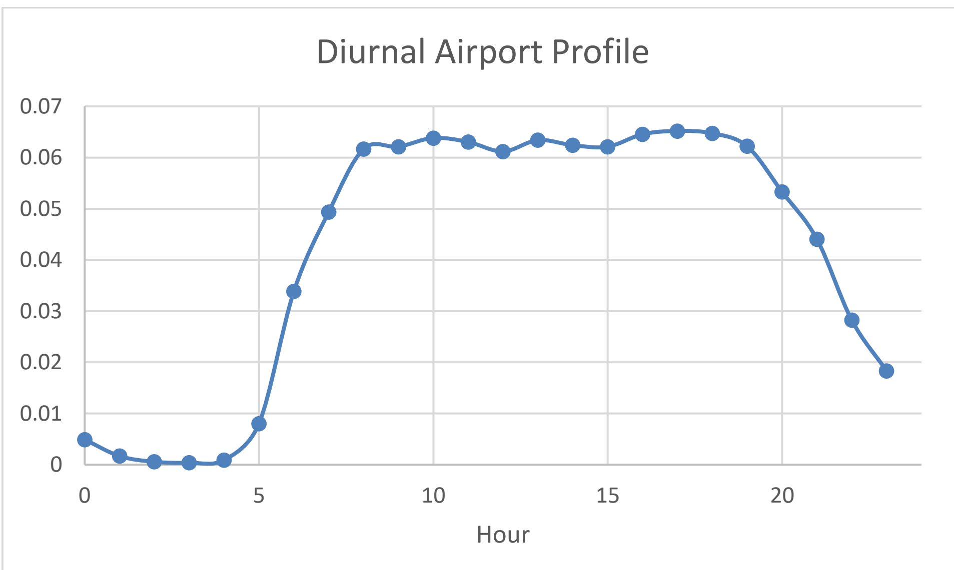


Figure 3-10. Weekly profile for all Airport SCCs

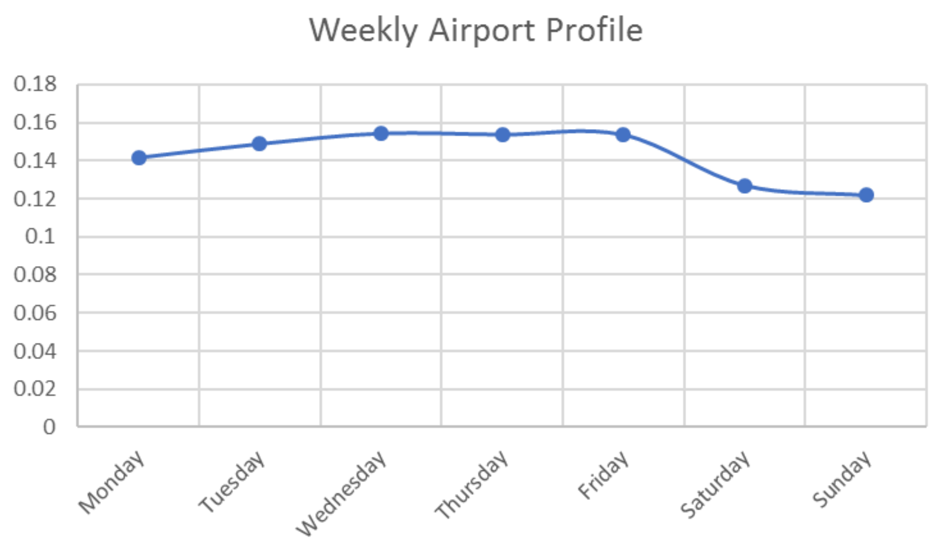


Figure 3-11. Monthly Profile for all Airport SCCs

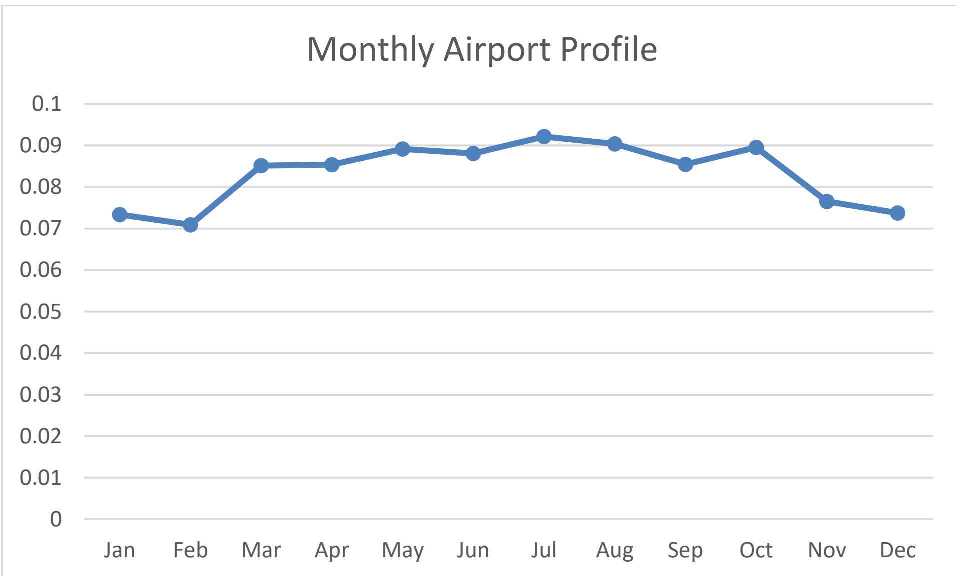
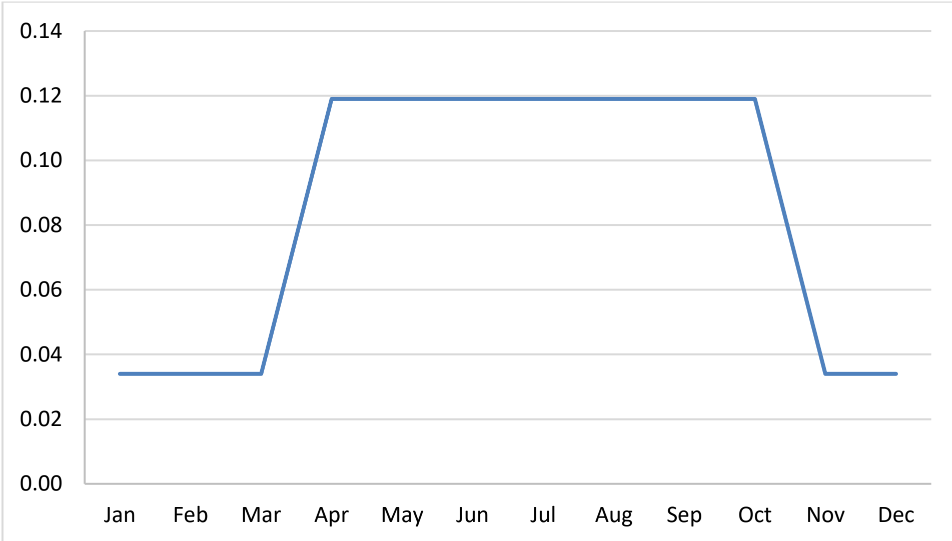


Figure 3-12. Alaska Seaplane Profile



3.3.4 Residential Wood Combustion Temporal allocation (rwc)

There are many factors that impact the timing of when emissions occur, and for some sectors this includes meteorology. The benefits of utilizing meteorology as a method for temporal allocation are: (1) a meteorological dataset consistent with that used by the AQ model is available (e.g., outputs from WRF); (2) the meteorological model data are highly resolved in terms of spatial resolution; and (3) the meteorological variables vary at hourly resolution and can, therefore, be translated into hour-specific temporal allocation.

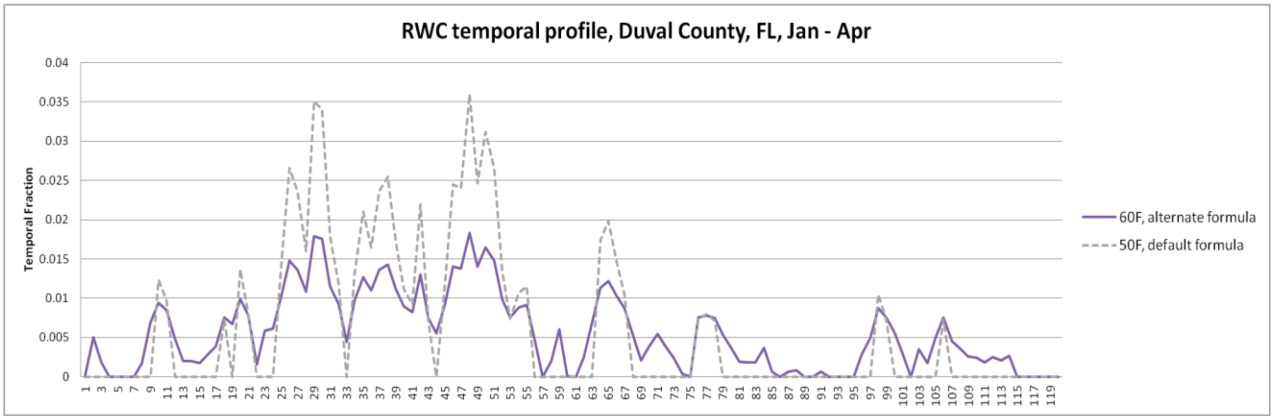
The SMOKE program Gentpro provides a method for developing meteorology-based temporal allocation. Currently, the program can utilize three types of temporal algorithms: annual-to-day temporal allocation for residential wood combustion (RWC); month-to-hour temporal allocation for agricultural livestock NH_3; and a generic meteorology-based algorithm for other situations. Meteorological-based temporal allocation was used for portions of the rwc sector and for the entire ag sector.

Gentpro reads in gridded meteorological data (output from MCIP) along with spatial surrogates, and uses the specified algorithm to produce a new temporal profile that can be input into SMOKE. The meteorological variables and the resolution of the generated temporal profile (hourly, daily, etc.) depend on the selected algorithm and the run parameters. For more details on the development of these algorithms and running Gentpro, see the Gentpro documentation and the SMOKE documentation at http://www.cmascenter.org/smoke/documentation/3.1/GenTPRO_TechnicalSummary_Aug2012_Final.pdf and https://www.cmascenter.org/smoke/documentation/4.5/html/ch05s03s05.html, respectively.

For the RWC algorithm, Gentpro uses the daily minimum temperature to determine the temporal allocation of emissions to days. Gentpro was used to create an annual-to-day temporal profile for the RWC sources. These generated profiles distribute annual RWC emissions to the coldest days of the year. On days where the minimum temperature does not drop below a user-defined threshold, RWC emissions for most sources in the sector are zero. Conversely, the program temporally allocates the largest percentage of emissions to the coldest days. Similar to other temporal allocation profiles, the total annual emissions do not change, only the distribution of the emissions within the year is affected. The temperature threshold for RWC emissions was 50 ˚F for most of the country, and 60 ˚F for the following states: Alabama, Arizona, California, Florida, Georgia, Louisiana, Mississippi, South Carolina, and Texas.

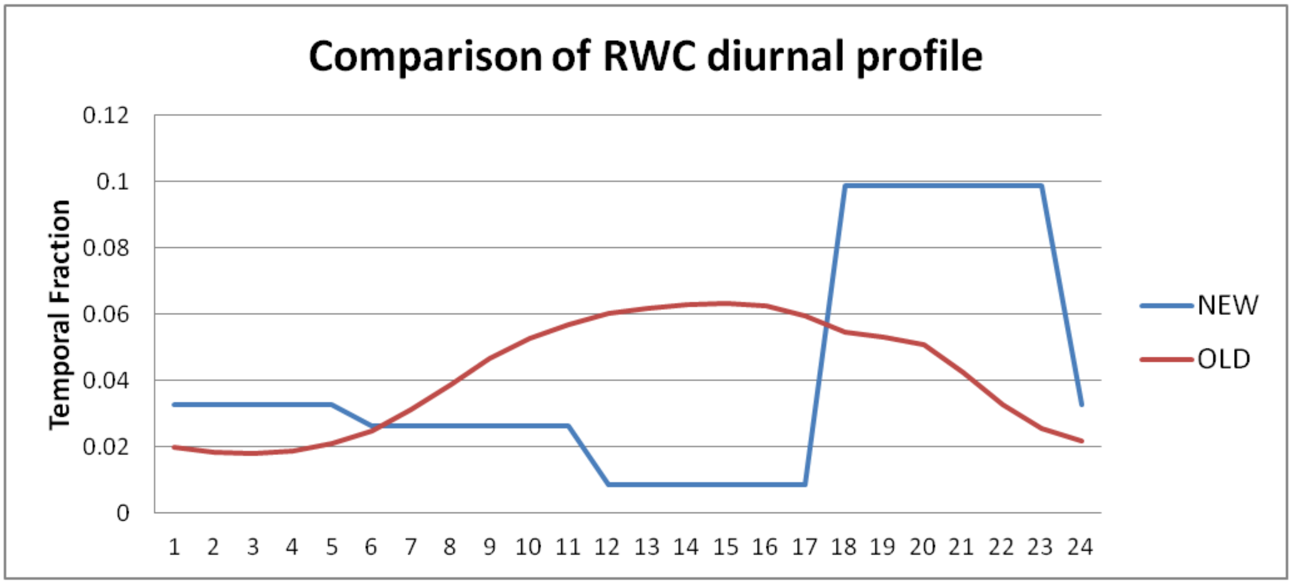
Figure 3-13 illustrates the impact of changing the temperature threshold for a warm climate county. The plot shows the temporal fraction by day for Duval County, Florida, for the first four months of 2007. The default 50 ˚F threshold creates large spikes on a few days, while the 60 ˚F threshold dampens these spikes and distributes a small amount of emissions to the days that have a minimum temperature between 50 and 60 ˚F.

Figure 3-13. Example of RWC temporal allocation in 2007 using a 50 versus 60 ˚F threshold



The diurnal profile for used for most RWC sources (see Figure 3-14) places more of the RWC emissions in the morning and the evening when people are typically using these sources. This profile is based on a 2004 MANE-VU survey based temporal profiles (see http://www.marama.org/publications_folder/ResWoodCombustion/Final_report.pdf). This profile was created by averaging three indoor and three RWC outdoor temporal profiles from counties in Delaware and aggregating them into a single RWC diurnal profile. This new profile was compared to a concentration-based analysis of aethalometer measurements in Rochester, New York (Wang *et al.* 2011) for various seasons and days of the week and was found that the new RWC profile generally tracked the concentration based temporal patterns.

Figure 3-14. RWC diurnal temporal profile



The temporal allocation for “Outdoor Hydronic Heaters” (i.e., “OHH,” SCC=2104008610) and “Outdoor wood burning device, NEC (fire-pits, chimneas, etc.)” (i.e., “recreational RWC,” SCC=21040087000) is not based on temperature data, because the meteorologically-based temporal allocation used for the rest of the rwc sector did not agree with observations for how these appliances are used.

For OHH, the annual-to-month, day-of-week and diurnal profiles were modified based on information in the New York State Energy Research and Development Authority’s (NYSERDA) “Environmental, Energy Market, and Health Characterization of Wood-Fired Hydronic Heater Technologies, Final Report” (NYSERDA, 2012), as well as a Northeast States for Coordinated Air Use Management (NESCAUM) report “Assessment of Outdoor Wood-fired Boilers” (NESCAUM, 2006). A Minnesota 2008 Residential Fuelwood Assessment Survey of individual household responses (MDNR, 2008) provided additional annual-to-month, day-of-week and diurnal activity information for OHH as well as recreational RWC usage.

The diurnal profile for OHH, shown in Figure 3-15, is based on a conventional single-stage heat load unit burning red oak in Syracuse, New York. As shown in Figure 3-16, the NESCAUM report describes how for individual units, OHH are highly variable day-to-day but that in the aggregate, these emissions have no day-of-week variation. In contrast, the day-of-week profile for recreational RWC follows a typical “recreational” profile with emissions peaked on weekends.

Annual-to-month temporal allocation for OHH as well as recreational RWC were computed from the MDNR 2008 survey and are illustrated in Figure 3-17. The OHH emissions still exhibit strong seasonal variability, but do not drop to zero because many units operate year-round for water and pool heating. In contrast to all other RWC appliances, recreational RWC emissions are used far more frequently during the warm season.

Figure 3-15. Diurnal profile for OHH, based on heat load (BTU/hr)

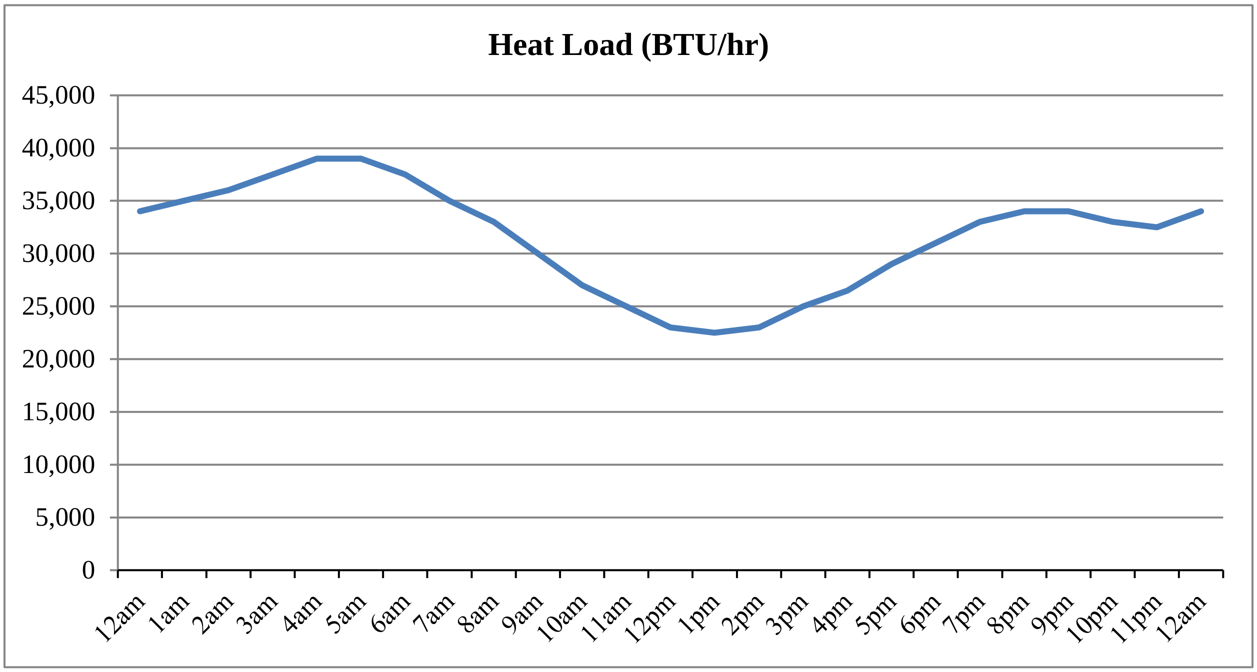


Figure 3-16. Day-of-week temporal profiles for OHH and Recreational RWC

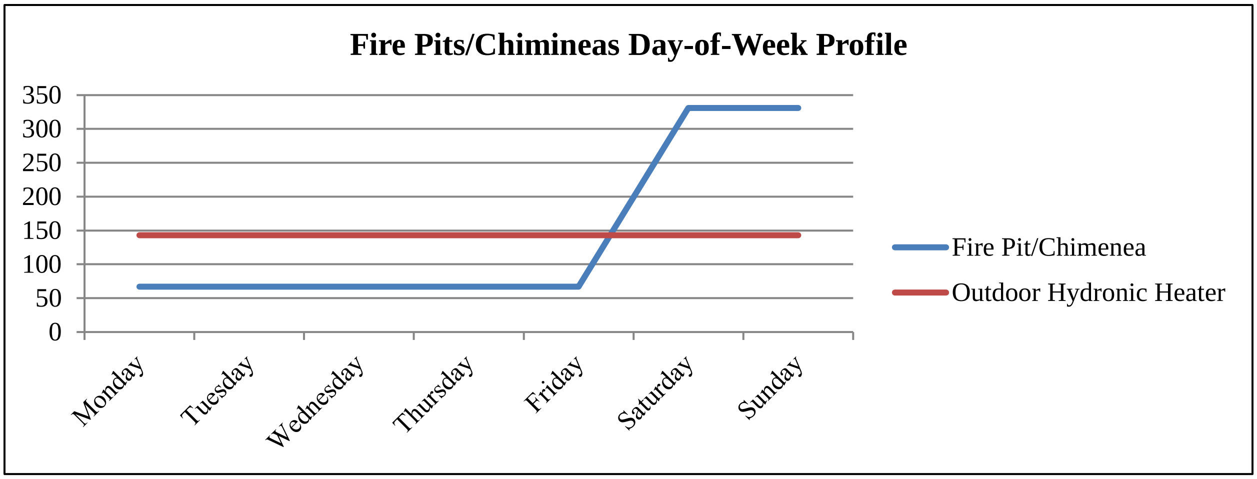
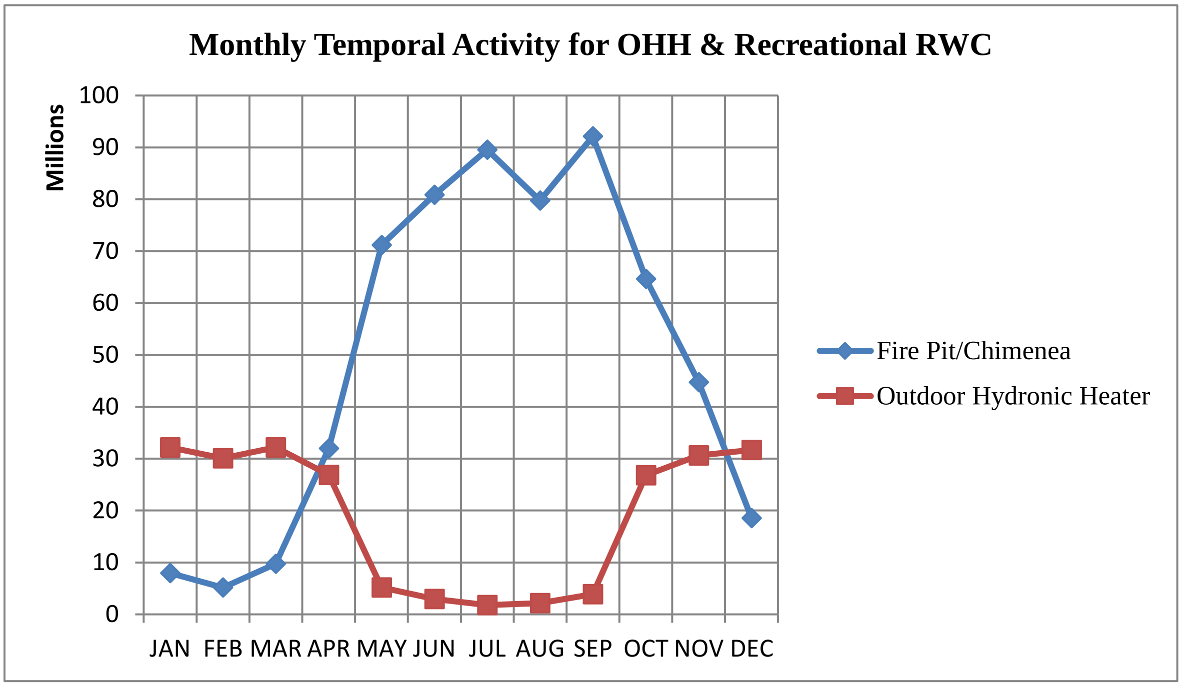


Figure 3-17. Annual-to-month temporal profiles for OHH and recreational RWC



3.3.5 Agricultural Ammonia Temporal Profiles (ag)

For the agricultural livestock NH_3 algorithm, the GenTPRO algorithm is based on an equation derived by Jesse Bash of the EPA's ORD based on the Zhu, Henze, et al. (2013) empirical equation. This equation is based on observations from the TES satellite instrument with the GEOS-Chem model and its adjoint to estimate diurnal NH_3 emission variations from livestock as a function of ambient temperature, aerodynamic resistance, and wind speed. The equations are:

$$E_{i,h} = [161500/T_{i,h} \text{ x } e^{(-1380/T_{i,h})}] \text{ x } AR_{i,h}$$

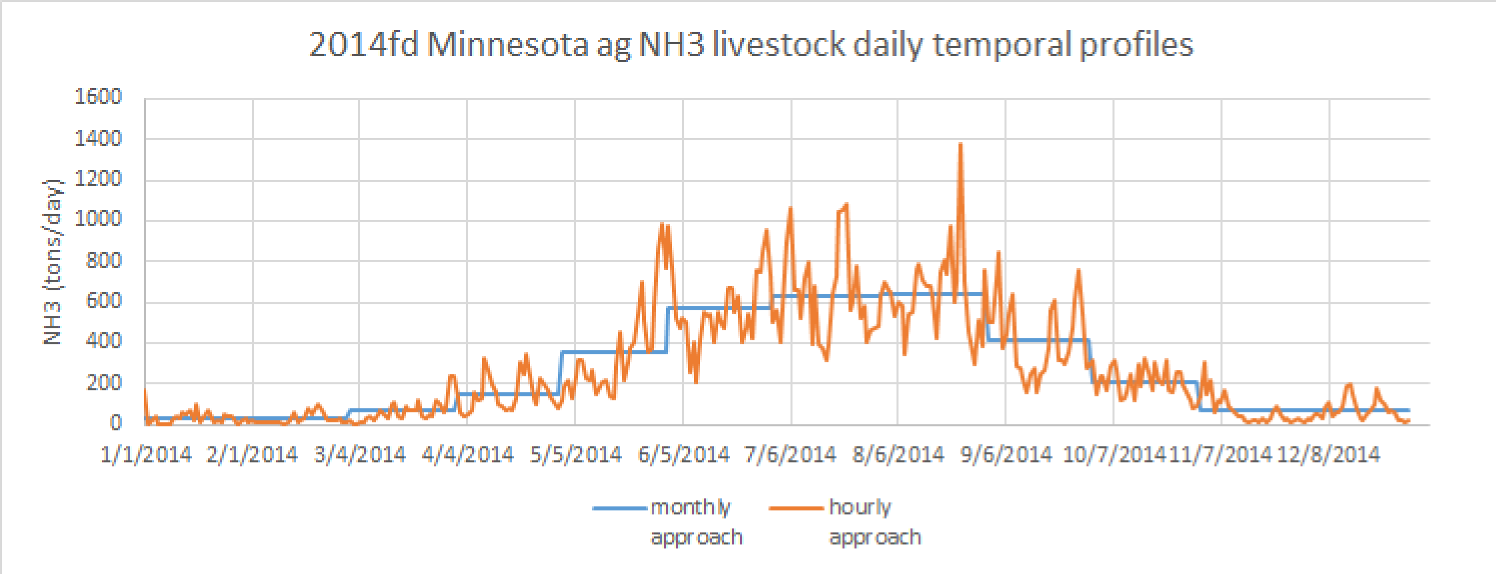
$$PE_{i,h} = E_{i,h} / \text{Sum}(E_{i,h})$$

where

- $PE_{i,h}$ = Percentage of emissions in county *i* on hour *h*
- $E_{i,h}$ = Emission rate in county *i* on hour *h*
- $T_{i,h}$ = Ambient temperature (Kelvin) in county *i* on hour *h*
- $V_{i,h}$ = Wind speed (meter/sec) in county *i* (minimum wind speed is 0.1 meter/sec)
- $AR_{i,h}$ = Aerodynamic resistance in county *i*

GenTPRO was run using the "BASH_NH3" profile method to create month-to-hour temporal profiles for these sources. Because these profiles distribute to the hour based on monthly emissions, the monthly emissions are obtained from a monthly inventory, or from an annual inventory that has been temporalized to the month. Figure 3-18 compares the daily emissions for Minnesota from the "old" approach (uniform monthly profile) with the "new" approach (GenTPRO generated month-to-hour profiles) for 2014. Although the GenTPRO profiles show daily (and hourly variability), the monthly total emissions are the same between the two approaches.

Figure 3-18. Example of animal NH_3 emissions temporal allocation approach, summed to daily emissions



For this 2015 platform, the GenTPRO approach is applied to all sources in the ag sector, NH_3 and non-NH_3, livestock and fertilizer. Monthly profiles are based on the daily-based EPA livestock emissions and are the same as were used in 2014v7.0. Profiles are by state/SCC_category, where SCC_category is one of the following: beef, broilers, layers, dairy, swine.

3.3.6 Oil and gas temporal allocation (np_oilgas)

For the 2014v7.1 platform, the monthly oil and gas temporal profiles by county and SCC were updated to use 2014 activity information. However, these profiles are based on year-specific activity which cannot necessarily be applied for other years such as 2015. Therefore, in the 2015 platform, the entire np_oilgas sector uses flat monthly temporalization. Weekly and diurnal profiles are flat and are based on comments received on a version of the 2011 platform.

3.3.7 Onroad mobile temporal allocation (onroad)

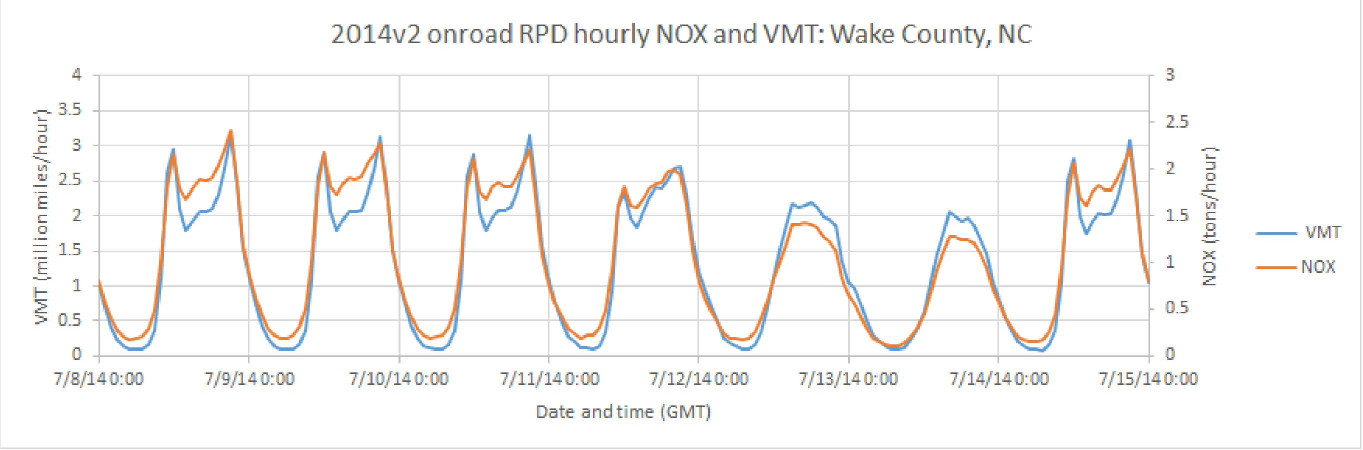
For the onroad sector, the temporal distribution of emissions is a combination of traditional temporal profiles and the influence of meteorology. This section will discuss both the meteorological influences and the development of the temporal profiles for this platform.

The "inventories" referred to in Table 3-18 consist of activity data for the onroad sector, not emissions. For the off-network emissions from the RPP and RPV processes, the VPOP activity data is annual and does not need temporal allocation. For processes that result from hoteling of combination trucks (RPH), the HOTELING inventory is annual and was temporalized to month, day of the week, and hour of the day through temporal profiles.

For on-roadway RPD processes, the VMT activity data is annual for some sources and monthly for other sources, depending on the source of the data. Sources without monthly VMT were temporalized from annual to month through temporal profiles. VMT was also temporalized from month to day of the week, and then to hourly through temporal profiles. The RPD processes require a speed profile (SPDPRO) that consists of vehicle speed by hour for a typical weekday and weekend day. For onroad, the temporal profiles and SPDPRO will impact not only the distribution of emissions through time but also the total emissions. Because SMOKE-MOVES (for RPD) calculates emissions based on the VMT, speed and meteorology, if one shifted the VMT or speed to different hours, it would align with different temperatures and hence different emission factors. In other words, two SMOKE-MOVES runs with identical annual VMT, meteorology, and MOVES emission factors, will have different total emissions if the temporal allocation of VMT changes. Figure 3-19 illustrates the temporal allocation of the onroad activity data (i.e., VMT) and the pattern of the emissions that result after running SMOKE-MOVES. In this figure, it can be seen that the meteorologically varying emission factors add variation on top of the temporal allocation of the activity data.

Meteorology is not used in the development of the temporal profiles, but rather it impacts the calculation of the hourly emissions through the program Movesmrg. The result is that the emissions vary at the hourly level by grid cell. More specifically, the on-network (RPD) and the off-network parked vehicle (RPV, RPH, and RPP) processes use the gridded meteorology (MCIP) either directly or indirectly. For RPD, RPV, and RPH, Movesmrg determines the temperature for each hour and grid cell and uses that information to select the appropriate emission factor for the specified SCC/pollutant/mode combination. For RPP, instead of reading gridded hourly meteorology, Movesmrg reads gridded daily minimum and maximum temperatures. The total of the emissions from the combination of these four processes (RPD, RPV, RPH, and RPP) comprise the onroad sector emissions. The temporal patterns of emissions in the onroad sector are influenced by meteorology.

Figure 3-19. Example of temporal variability of NO_X emissions



New VMT day-of-week and hour-of-day temporal profiles were developed for use in the 2014NEIv2 and later platforms as part of the effort to update the inputs to MOVES and SMOKE-MOVES under CRC A-100 (Coordinating Research Council, 2017). CRC A-100 data includes profiles by region or county, road type, and broad vehicle category. There are three vehicle categories: passenger vehicles (11/21/31), commercial trucks (32/52), and combination trucks (53/61/62). CRC A-100 does not cover buses, refuse trucks, or motor homes, so those vehicle types were mapped to other vehicle types for which CRC A-100 did provide profiles as follows: 1) Intercity/transit buses were mapped to commercial trucks; 2) Motor homes were mapped to passenger vehicles for day-of-week and commercial trucks for hour-of-day; 3) School buses and refuse trucks were mapped to commercial trucks for hour-of-day and use a new custom day-of-week profile called LOWSATSUN that has a very low weekend allocation, since school buses and refuse trucks operate primarily on business days. In addition to temporal profiles, CRC A-100 data were also used to develop the average hourly speed data (SPDPRO) used by SMOKE-MOVES. In areas where CRC A-100 data does not exist, hourly speed data is based on MOVES county databases.

The CRC A-100 dataset includes temporal profiles for individual counties, Metropolitan Statistical Areas (MSAs), and entire regions (e.g. West, South). For counties without county or MSA temporal profiles specific to itself, regional temporal profiles are used. Temporal profiles also vary by each of the MOVES road types, and there are distinct hour-of-day profiles for each day of the week. Plots of hour-of-day profiles for passenger vehicles in Fulton County, GA, are shown in Figure 3-20. Separate plots are shown for Monday, Friday, Saturday, and Sunday, and each line corresponds to a particular MOVES road type (i.e.,. road type 2 = rural restricted, 3 = rural unrestricted, 4 = urban restricted, and 5 = urban unrestricted). Figure 3-21 shows which counties have temporal profiles specific to that county, and which counties use regional average profiles.

Figure 3-20. Sample onroad diurnal profiles for Fulton County, GA

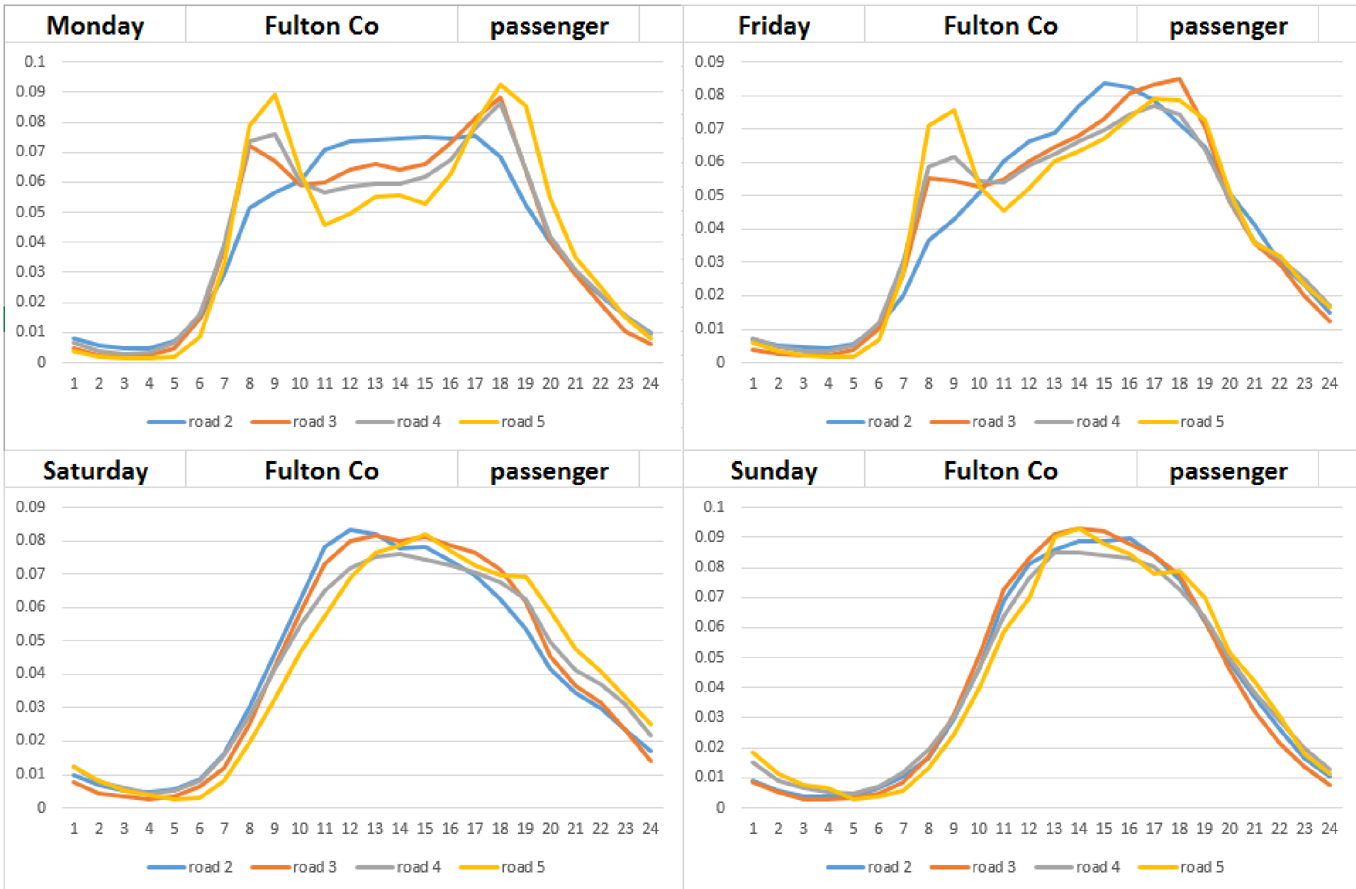
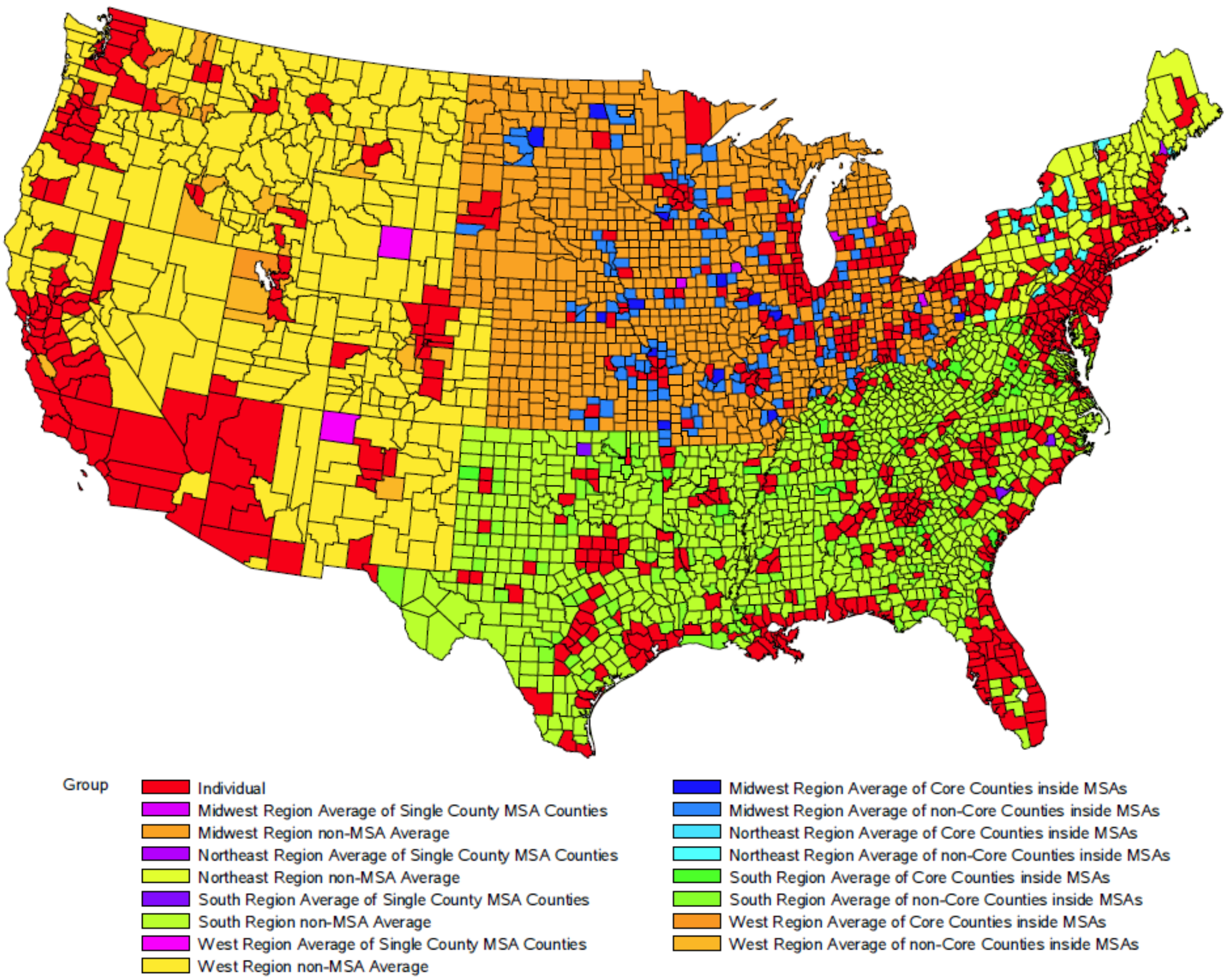


Figure 3-21. Counties for which MOVES Speeds and Temporal Profiles could be Populated

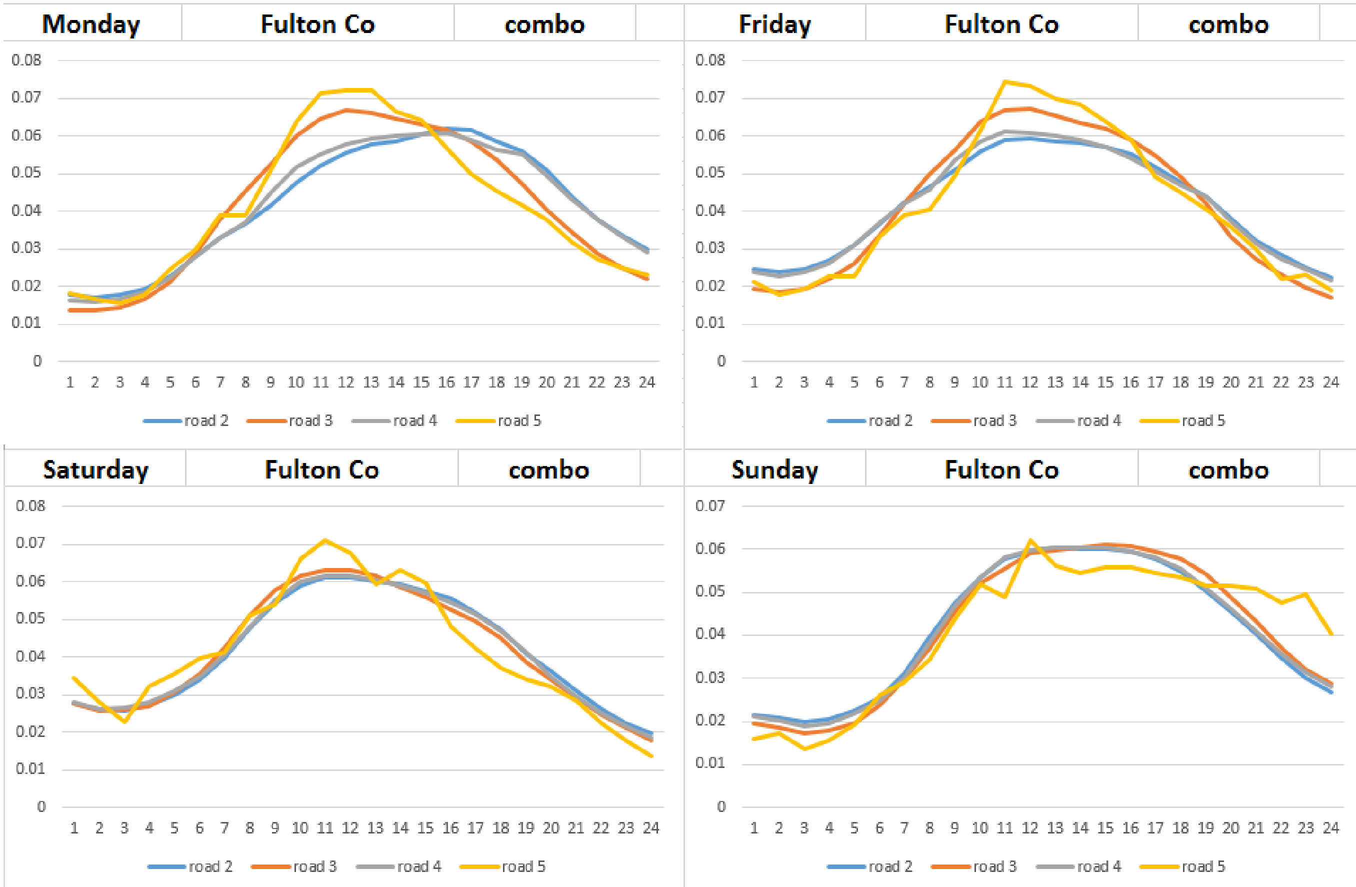


For hoteling, day-of-week profiles are the same as non-hoteling for combination trucks, while hour-of-day non-hoteling profiles for combination trucks were inverted to create new hoteling profiles that peak overnight instead of during the day. The combination truck profiles for Fulton County are shown in Figure 3-22.

The CRC A-100 temporal profiles were used in the entire contiguous United States, except in California. All California temporal profiles were carried over from 2014v7.0, although California hoteling uses CRC A-100-based profiles just like the rest of the country, since CARB didn't have a hoteling-specific profile. Monthly profiles in all states (national profiles by broad vehicle type) were also carried over from 2014v7.0 and applied directly to the VMT. For California, CARB supplied diurnal profiles that varied by vehicle type, day of the week[15], and air basin. These CARB-specific profiles were used in developing EPA estimates for California. Although the EPA adjusted the total emissions to match California-submitted emissions, the temporal allocation of these emissions took into account both the state-specific VMT profiles and the SMOKE-MOVES process of incorporating meteorology. For more details on the adjustments to California's onroad emissions, see Section 2.3.1.

[15] California's diurnal profiles varied within the week. Monday, Friday, Saturday, and Sunday had unique profiles and Tuesday, Wednesday, Thursday had the same profile.

Figure 3-22. Example of Temporal Profiles for Combination Trucks



3.3.8 Additional sector specific details (afdust, beis, cmv, rail, nonpt, ptnonipm, ptfire)

For the afdust sector, meteorology is not used in the development of the temporal profiles, but it is used to reduce the total emissions based on meteorological conditions. These adjustments are applied through sector-specific scripts, beginning with the application of land use-based gridded transport fractions and then subsequent zero-outs for hours during which precipitation occurs or there is snow cover on the ground. The land use data used to reduce the NEI emissions explains the amount of emissions that are subject to transport. This methodology is discussed in (Pouliot et al., 2010, http://www3.epa.gov/ttn/chief/conference/ei19/session9/pouliot_pres.pdf), and in "Fugitive Dust Modeling for the 2008 Emissions Modeling Platform" (Adelman, 2012). The precipitation adjustment is applied to remove all emissions for hours where measurable rain occurs, or where there is snow cover. Therefore, the afdust emissions vary day-to-day based on the precipitation and/or snow cover for each grid cell and hour. Both the transport fraction and meteorological adjustments are based on the gridded resolution of the platform; therefore, somewhat different emissions will result for different grid resolutions.

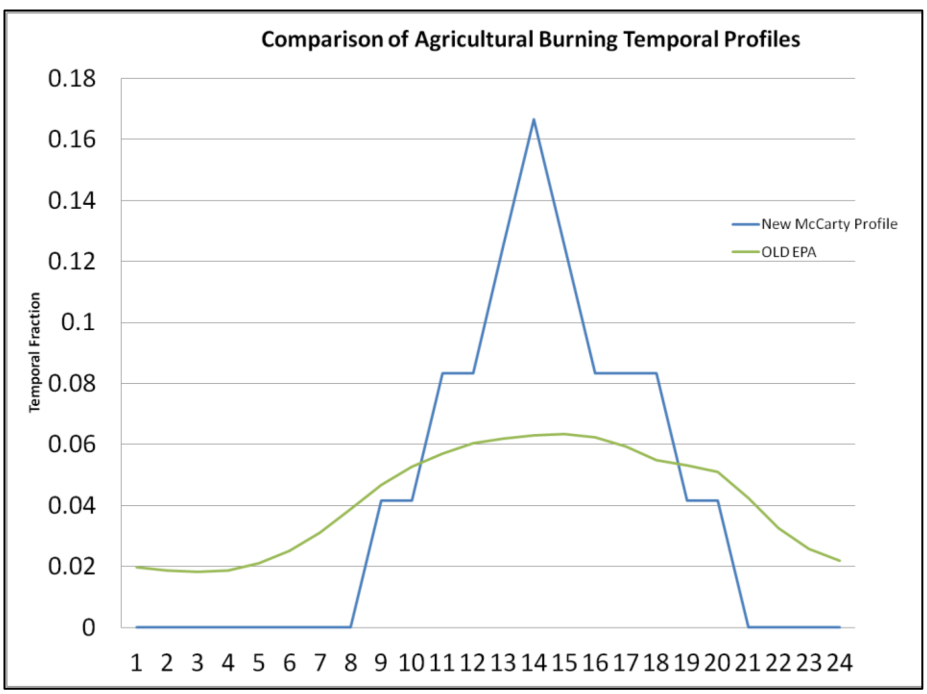
Biogenic emissions in the beis sector vary by every day of the year because they are developed using meteorological data including temperature, surface pressure, and radiation/cloud data. The emissions are computed using appropriate emission factors according to the vegetation in each model grid cell, while taking the meteorological data into account.

For the cmv sectors, emissions are allocated with flat day of week and flat hourly profiles. Updated monthly profiles were developed for the LADCO states using link-level NO_X emissions for ship traffic provided by LADCO. These data were based on activities reported by ship AIS (transponder) devices. Monthly NOx emissions were normalized to create temporal profiles for each lake. For the port SCCs, an in-port profile was developed as the average of the maneuvering and hoteling emissions. The cruising emissions were used for the underway SCCs. As some of the lakes did not include complete data for the in-port sources (Ontario, Canada, St. Claire), a hybrid profile was created as an average of the in-port NOx emissions for Lakes Michigan, Huron, Superior, and Erie. A resulting 22 profiles were developed and applied to C1, C2 and C3 ships based county and SCC (i.e., port versus underway). Only new monthly profiles were developed from these data because the weekly and diurnal variation were deemed to be comparable to the existing EPA profiles. For non-LADCO areas, C1 and C2 monthly profiles are flat and C3 monthly profiles are highest (but not significantly different from the rest of the year) in the summer.

For the rail sector, new monthly profiles were developed for the 2014 platform. Monthly temporal allocation for rail freight emissions is based on AAR Rail Traffic Data, Total Carloads and Intermodal, for 2014. For passenger trains, monthly temporal allocation is based on rail passenger miles data for 2014 from the Bureau of Transportation Statistics. Rail emissions are allocated with flat day of week profiles, and most emissions are allocated with flat hourly profiles. These 2014-based profiles are used for the 2015 modeling.

For the ptagfire sector, the inventories are in the daily point fire format FF10 PTDAY. The diurnal temporal profile for ag fires reflects the fact that burning occurs during the daylight hours - see Figure 3-23 (McCarty et al., 2009). This puts most of the emissions during the work day and suppresses the emissions during the middle of the night.

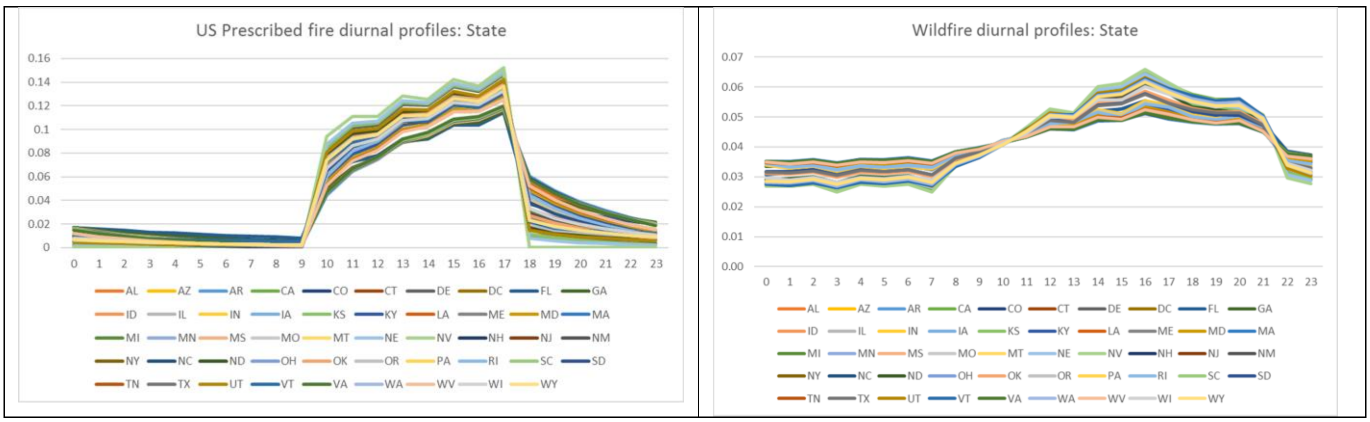
Figure 3-23. Agricultural burning diurnal temporal profile



Industrial processes that are not likely to shut down on Sundays, such as those at cement plants, use profiles that include emissions on Sundays, while those that would shut down on Sundays use profiles that reflect Sunday shutdowns.

For the ptfire sectors, the inventories are in the daily point fire format FF10 PTDAY. Separate hourly profiles for prescribed and wildfires were used. Figure 3-24 below shows the profiles used for each state for the 2014v7.0 and 2014v7.1 modeling platforms. They are similar but not the same and vary according to the average meteorological conditions in each state. The 2015 platform uses the same ptfire diurnal as the 2014v7.1 platform.

Figure 3-24. Prescribed and Wildfire diurnal temporal profiles



For the nonroad sector, while the NEI only stores the annual totals, the modeling platform uses monthly inventories from output from MOVES. For California, CARB's annual inventory was temporalized to monthly using monthly temporal profiles applied in SMOKE by SCC. This is an improvement over the 2011 platform, which applied monthly temporal allocation in California at the broader SCC7 level.

3.4 Spatial Allocation

The methods used to perform spatial allocation are summarized in this section. For the modeling platform, spatial factors are typically applied by county and SCC. As described in Section 3.1, spatial allocation was performed for the larger 12-km U.S. domain. To accomplish this, SMOKE used national 12-km spatial surrogates and a SMOKE area-to-point data file. For the U.S., the EPA updated surrogates to use circa 2014 data wherever possible. For Mexico, updated spatial surrogates were used as described below. For Canada, updated surrogates were provided by Environment Canada for 2014v7.1. The U.S., Mexican, and Canadian 12-km surrogates cover the entire CONUS domain 12US1 shown in Figure 3-1.

Documentation of the origin of the spatial surrogates for the platform is provided in the workbook US_SpatialSurrogate_Workbook_v07172018 which is available with the reports for the 2014v7.1 platform. The remainder of this subsection summarizes the data used for the spatial surrogates and the area-to-point data which is used for airport refueling.

3.4.1 Spatial Surrogates for U.S. emissions

There are more than 100 spatial surrogates available for spatially allocating U.S. county-level emissions to the 36-km and 12-km grid cells used by the air quality model. As described in Section 3.4.2, an area-to-point approach overrides the use of surrogates for a airport refueling sources. Table 3-19 lists the codes and descriptions of the surrogates. Surrogate names and codes listed in *italics* are not directly assigned to any sources for the 2015 platform, but they are sometimes used to gapfill other surrogates, or as an input for merging two surrogates to create a new surrogate that is used.

Many surrogates were updated or newly developed for use in the 2014v7.0 platform (Adelman, 2016). They include the use of the 2011 National Land Cover Database (the previous platform used 2006) and development of various development density levels such as open, low, medium high and various combinations of these. These landuse surrogates largely replaced the FEMA category surrogates that were used in the 2011 platform. Additionally, onroad surrogates were developed using average annual daily traffic counts from the highway monitoring performance system (HPMS). Previously, the "activity" for the onroad surrogates was length of road miles. This and other surrogates are described in a reference (Adelman, 2016).

Several surrogates were updated or developed as new surrogates for 2014v7.1, and used in 2015 platform:

- c1/c2 ships at ports uses a surrogate based on 2014 NEI ports activity data based on use of the 2014NEIv1 (surrogate 820); previously, just the port shapes (801) were used.
- c1/c2 ships underway uses a 2013-shipping density surrogate (surrogate 808); previously Offshore Shipping NEI2014 Activity (806) was used.
- Oil and gas surrogates were updated to correct errors found after they were used for 2014v7.0;
- Onroad spatial allocation uses surrogates that do not distinguish between urban and rural road types, correcting the issue arising in some counties due to the inconsistent urban and rural definitions between MOVES and the surrogate data;
- Correction was made to the water surrogate to gap fill missing counties using 2006 NLCD.

The surrogates for the U.S. were mostly generated using the Surrogate Tool to drive the Spatial Allocator, but a few surrogates were developed directly within ArcGIS or using scripts that manipulate spatial data in PostgreSQL . The tool and documentation for the Surrogate Tool is available at https://www.cmascenter.org/sa-tools/documentation/4.2/SurrogateToolUserGuide_4_2.pdf.

Table 3-19. U.S. Surrogates available for the 2015 modeling platform

Code	Surrogate Description	Code	Surrogate Description
N/A	Area-to-point approach (see 3.6.2)	505	Industrial Land
100	Population	506	Education
110	*Housing*	*507*	*Heavy Light Construction Industrial Land*
131	*urban Housing*	*510*	*Commercial plus Industrial*
132	*Suburban Housing*	*515*	*Commercial plus Institutional Land*
134	*Rural Housing*	*520*	*Commercial plus Industrial plus Institutional*
137	*Housing Change*	*525*	*Golf Courses plus Institutional plus Industrial plus Commercial*
140	*Housing Change and Population*	*526*	*Residential – Non-Institutional*

Code	Surrogate Description	Code	Surrogate Description
150	Residential Heating – Natural Gas	*527*	*Single Family Residential*
160	*Residential Heating – Wood*	535	Residential + Commercial + Industrial + Institutional + Government
170	Residential Heating – Distillate Oil	*540*	*Retail Trade (COM1)*
180	Residential Heating – Coal	*545*	*Personal Repair (COM3)*
190	Residential Heating – LP Gas	*555*	*Professional/Technical (COM4) plus General Government (GOV1)*
201	*Urban Restricted Road Miles*	560	Hospital (COM6)
202	Urban Restricted AADT	*575*	*Light and High Tech Industrial (IND2 + IND5)*
205	Extended Idle Locations	*580*	*Food Drug Chemical Industrial (IND3)*
211	*Rural Restricted Road Miles*	*585*	*Metals and Minerals Industrial (IND4)*
212	*Rural Restricted AADT*	*590*	*Heavy Industrial (IND1)*
221	*Urban Unrestricted Road Miles*	*595*	*Light Industrial (IND2)*
222	*Urban Unrestricted AADT*	*596*	*Industrial plus Institutional plus Hospitals*
231	*Rural Unrestricted Road Miles*	650	Refineries and Tank Farms
232	*Rural Unrestricted AADT*	670	Spud Count – CBM Wells
239	Total Road AADT	671	Spud Count – Gas Wells
240	Total Road Miles	672	Gas Production at Oil Wells
241	*Total Restricted Road Miles*	673	Oil Production at CBM Wells
242	All Restricted AADT	674	Unconventional Well Completion Counts
243	*Total Unrestricted Road Miles*	*676*	*Well Count – All Producing*
244	All Unrestricted AADT	*677*	*Well Count – All Exploratory*
258	Intercity Bus Terminals	678	Completions at Gas Wells
259	Transit Bus Terminals	679	Completions at CBM Wells
260	*Total Railroad Miles*	681	Spud Count – Oil Wells
261	NTAD Total Railroad Density	683	Produced Water at All Wells
271	NTAD Class 1 2 3 Railroad Density	685	Completions at Oil Wells
272	*NTAD Amtrak Railroad Density*	*686*	*Completions at All Wells*
273	*NTAD Commuter Railroad Density*	687	Feet Drilled at All Wells
275	*ERTAC Rail Yards*	691	Well Counts - CBM Wells
280	*Class 2 and 3 Railroad Miles*	692	Spud Count – All Wells
300	NLCD Low Intensity Development	693	Well Count – All Wells
301	*NLCD Med Intensity Development*	694	Oil Production at Oil Wells
302	*NLCD High Intensity Development*	695	Well Count – Oil Wells
303	*NLCD Open Space*	696	Gas Production at Gas Wells
304	NLCD Open + Low	697	Oil Production at Gas Wells
305	NLCD Low + Med	698	Well Count – Gas Wells
306	NLCD Med + High	699	Gas Production at CBM Wells
307	NLCD All Development	*710*	*Airport Points*
308	NLCD Low + Med + High	711	Airport Areas
309	NLCD Open + Low + Med	801	Port Areas
310	NLCD Total Agriculture	*805*	*Offshore Shipping Area*
318	*NLCD Pasture Land*	*806*	*Offshore Shipping NEI2014 Activity*
319	NLCD Crop Land	*807*	*Navigable Waterway Miles*
320	NLCD Forest Land	808	2013 Shipping Density
321	NLCD Recreational Land	820	Ports NEI2014 Activity
340	*NLCD Land*	850	Golf Courses
350	NLCD Water	860	Mines

Code	Surrogate Description	Code	Surrogate Description
500	*Commercial Land*	*890*	*Commercial Timber*

For the onroad sector, the on-network (RPD) emissions were allocated differently from the off-network (RPP and RPV). On-network used average annual daily traffic (AADT) data and off network used land use surrogates as shown in Table 3-20. Emissions from the extended (i.e., overnight) idling of trucks were assigned to surrogate 205, which is based on locations of overnight truck parking spaces. This surrogate's underlying data were updated for use in the 2014 and 2015 platforms to include additional data sources and corrections based on comments received on the 2011 NATA.

Table 3-20. Off-Network Mobile Source Surrogates

Source type	Source Type name	**Surrogate ID**	**Description**
11	Motorcycle	307	NLCD All Development
21	Passenger Car	307	NLCD All Development
31	Passenger Truck	307	NLCD All Development
32	Light Commercial Truck	308	NLCD Low + Med + High
41	Intercity Bus	258	Intercity Bus Terminals
42	Transit Bus	259	Transit Bus Terminals
43	School Bus	506	Education
51	Refuse Truck	306	NLCD Med + High
52	Single Unit Short-haul Truck	306	NLCD Med + High
53	Single Unit Long-haul Truck	306	NLCD Med + High
54	Motor Home	304	NLCD Open + Low
61	Combination Short-haul Truck	306	NLCD Med + High
62	Combination Long-haul Truck	306	NLCD Med + High

For the oil and gas sources in the np_oilgas sector, the spatial surrogates were updated to those shown in Table 3-21 using 2014 data consistent with what was used to develop the 2014NEI nonpoint oil and gas emissions. The primary activity data source used for the development of the oil and gas spatial surrogates was data from Drilling Info (DI) Desktop's HPDI database (Drilling Info, 2015). This database contains well-level location, production, and exploration statistics at the monthly level.
Due to a proprietary agreement with DI Desktop, individual well locations and ancillary production cannot be made publicly available, but aggregated statistics are allowed. These data were supplemented with data from state Oil and Gas Commission (OGC) websites (Illinois, Idaho, Indiana, Kentucky, Missouri, Nevada, Oregon and Pennsylvania, Tennessee). In many cases, the correct surrogate parameter was not available (e.g., feet drilled), but an alternative surrogate parameter was available (e.g., number of spudded wells) and downloaded. Under that methodology, both completion date and date of first production from HPDI were used to identify wells completed during 2011. In total, over 1.43 million unique wells were compiled from the above data sources. The wells cover 34 states and 1,158 counties. (ERG, 2016b). Corrections to these data were made for the 2014v7.1 platform, and carried forward into the 2015 platform, after errors were discovered in some counties.

Table 3-21. Spatial Surrogates for Oil and Gas Sources

Surrogate Code	Surrogate Description
670	Spud Count - CBM Wells
671	Spud Count - Gas Wells
672	Gas Production at Oil Wells
673	Oil Production at CBM Wells
674	Unconventional Well Completion Counts
676	Well Count - All Producing
677	Well Count - All Exploratory
678	Completions at Gas Wells
679	Completions at CBM Wells
681	Spud Count - Oil Wells
683	Produced Water at All Wells
685	Completions at Oil Wells
686	Completions at All Wells
687	Feet Drilled at All Wells
691	Well Counts - CBM Wells
692	Spud Count - All Wells
693	Well Count - All Wells
694	Oil Production at Oil Wells
695	Well Count - Oil Wells
696	Gas Production at Gas Wells
697	Oil Production at Gas Wells
698	Well Count - Gas Wells
699	Gas Production at CBM Wells

Not all of the available surrogates are used to spatially allocate sources in the modeling platform; that is, some surrogates shown in Table 3-19 were not assigned to any SCCs, although many of the “unused” surrogates are actually used to “gap fill” other surrogates that are used. When the source data for a surrogate has no values for a particular county, gap filling is used to provide values for the surrogate in those counties to ensure that no emissions are dropped when the spatial surrogates are applied to the emission inventories. Table 3-22 shows the CAP emissions (i.e., NH_3, NOx, $PM_{2.5}$, SO_2, and VOC) by sector assigned to each spatial surrogate.

Table 3-22. Selected 2015 CAP emissions by sector for U.S. Surrogates (12US1 domain totals)

Sector	ID	Description	NH3	NOX	PM2_5	SO2	VOC
Afdust	240	Total Road Miles			283,210		
Afdust	304	NLCD Open + Low			1,053,145		
Afdust	306	NLCD Med + High			43,636		
Afdust	308	NLCD Low + Med + High			122,943		
Afdust	310	NLCD Total Agriculture			987,447		
Ag	310	NLCD Total Agriculture	2,823,395				179,970
cmv_c1c2	808	2013 Shipping Density	293	520,571	14,357	4,207	9,117
cmv_c1c2	820	Ports NEI2014 Activity	11	23,201	729	1,482	972
nonpt	100	Population	32,842	0	0	0	1,222,980
nonpt	150	Residential Heating - Natural Gas	47,819	227,291	3,837	1,494	13,756
nonpt	170	Residential Heating - Distillate Oil	1,861	35,101	3,978	56,026	1,241
nonpt	180	Residential Heating - Coal	20	101	53	1,086	111
nonpt	190	Residential Heating - LP Gas	121	34,432	183	762	1,332
nonpt	239	Total Road AADT	0	25	551	0	274,177
nonpt	240	Total Road Miles	0	0	0	0	34,027
nonpt	242	All Restricted AADT	0	0	0	0	5,451
nonpt	244	All Unrestricted AADT	0	0	0	0	95,292
nonpt	271	NTAD Class 1 2 3 Railroad Density	0	0	0	0	2,252
nonpt	300	NLCD Low Intensity Development	5,184	27,632	103,906	3,720	74,580
nonpt	304	NLCD Open + Low	0	0	0	0	0
nonpt	306	NLCD Med + High	28,046	200,320	238,731	65,131	948,148
nonpt	307	NLCD All Development	24	46,331	126,722	14,185	596,598
nonpt	308	NLCD Low + Med + High	1,166	185,948	16,915	19,736	65,608
nonpt	310	NLCD Total Agriculture	0	0	37	0	204,819
nonpt	319	NLCD Crop Land	0	0	95	71	293
nonpt	320	NLCD Forest Land	4,143	378	1,289	9	474
nonpt	505	Industrial Land	0	0	0	0	174
nonpt	535	Residential + Commercial + Industrial + Institutional + Government	5	2	130	0	39
nonpt	560	Hospital (COM6)	0	0	0	0	0
nonpt	650	Refineries and Tank Farms	0	22	0	0	98,989
nonpt	711	Airport Areas	0	0	0	0	282
nonpt	801	Port Areas	0	0	0	0	8,059
nonroad	261	NTAD Total Railroad Density	3	2,584	272	4	500
nonroad	304	NLCD Open + Low	4	2,199	191	6	3,230
nonroad	305	NLCD Low + Med	110	22,782	4,549	146	148,910
nonroad	306	NLCD Med + High	339	240,678	15,532	522	124,752
nonroad	307	NLCD All Development	101	35,965	15,347	132	168,805
nonroad	308	NLCD Low + Med + High	662	454,115	37,672	874	68,825
nonroad	309	NLCD Open + Low + Med	111	22,100	1,249	148	44,312
nonroad	310	NLCD Total Agriculture	475	416,654	31,718	664	47,528
nonroad	320	NLCD Forest Land	19	8,705	1,332	24	8,317

Sector	ID	Description	NH3	NOX	PM2_5	SO2	VOC
nonroad	321	NLCD Recreational Land	157	20,730	15,115	226	553,559
nonroad	350	NLCD Water	215	143,603	8,628	361	447,354
nonroad	850	Golf Courses	13	2,149	115	17	5,662
nonroad	860	Mines	2	2,760	298	4	549
np_oilgas	670	Spud Count - CBM Wells	0	0	0	0	179
np_oilgas	671	Spud Count - Gas Wells	0	0	0	0	10,213
np_oilgas	672	Gas Production at Oil Wells	0	3,114	0	21,703	132,924
np_oilgas	673	Oil Production at CBM Wells	0	60	0	0	3,510
np_oilgas	674	Unconventional Well Completion Counts	0	49,995	1,793	237	3,633
np_oilgas	678	Completions at Gas Wells	0	3,598	26	6,768	71,380
np_oilgas	679	Completions at CBM Wells	0	13	0	483	1,581
np_oilgas	681	Spud Count - Oil Wells	0	0	0	0	71,799
np_oilgas	683	Produced Water at All Wells	0	12	0	0	96,489
np_oilgas	685	Completions at Oil Wells	0	3,526	129	2,266	55,417
np_oilgas	687	Feet Drilled at All Wells	0	119,951	3,995	449	9,569
np_oilgas	691	Well Counts - CBM Wells	0	32,515	483	12	27,146
np_oilgas	692	Spud Count - All Wells	0	9,020	255	113	366
np_oilgas	693	Well Count - All Wells	0	0	0	0	191
np_oilgas	694	Oil Production at Oil Wells	0	5,446	0	6,337	1,148,869
np_oilgas	695	Well Count - Oil Wells	0	121,851	2,892	80	452,987
np_oilgas	696	Gas Production at Gas Wells	0	48,679	2,123	163	56,273
np_oilgas	697	Oil Production at Gas Wells	0	1,405	0	25	379,201
np_oilgas	698	Well Count - Gas Wells	15	318,258	5,457	299	679,839
np_oilgas	699	Gas Production at CBM Wells	0	2,489	325	26	4,837
onroad	205	Extended Idle Locations	509	182,233	2,501	73	35,634
onroad	239	Total Road AADT					6,780
onroad	242	All Restricted AADT	36,812	1,414,639	45,066	8,378	226,757
onroad	244	All Unrestricted AADT	67,151	2,138,188	82,736	17,676	590,047
onroad	258	Intercity Bus Terminals		153	2	0	35
onroad	259	Transit Bus Terminals		100	4	0	222
onroad	304	NLCD Open + Low		779	19	1	2,595
onroad	306	NLCD Med + High		15,884	317	18	18,741
onroad	307	NLCD All Development		608,367	12,902	965	1,253,173
onroad	308	NLCD Low + Med + High		40,355	744	62	64,388
onroad	506	Education		545	21	1	835
rail	261	NTAD Total Railroad Density	4	15,222	368	286	873
rail	271	NTAD Class 1 2 3 Railroad Density	359	657,335	18,786	415	33,866
rwc	300	NLCD Low Intensity Development	15,331	30,493	313,945	7,684	338,465

3.4.2 Allocation method for airport-related sources in the U.S.

There are numerous airport-related emission sources in the NEI, such as aircraft, airport ground support equipment, and jet refueling. The modeling platform includes the aircraft and airport ground support equipment emissions as point sources. For the modeling platform, the EPA used the SMOKE "area-to-point" approach for only jet refueling in the nonpt sector. The following SCCs use this approach: 2501080050 and 2501080100 (petroleum storage at airports), and 2810040000 (aircraft/rocket engine firing and testing). The ARTOPNT approach is described in detail in the 2002 platform documentation: http://www3.epa.gov/scram001/reports/Emissions%20TSD%20Vol1_02-28-08.pdf. The ARTOPNT file that lists the nonpoint sources to locate using point data were unchanged from the 2005-based platform.

3.4.3 Surrogates for Canada and Mexico emission inventories

Spatial surrogates for allocating Canada and Mexico province/sub-province and municipio level emissions were updated in the 2014v7.1 platform and carried forward into the 2015 platform. A new set of Canada shapefiles were provided by Environment Canada along with cross references spatially allocate the new 2013 Canadian emissions. Gridded surrogates were generated using the Surrogate Tool (previously referenced); Table 3-23 provides a list. Due to computational reasons, total roads (1263) were used instead of the unpaved rural road surrogate provided. The population surrogate was recently updated for Mexico; surrogate code 11, which uses 2015 population data at 1 km resolution, replaces the previous population surrogate code 10. The other surrogates for Mexico are circa 1999 and 2000 and were based on data obtained from the Sistema Municpal de Bases de Datos (SIMBAD) de INEGI and the Bases de datos del Censo Economico 1999. Most of the CAPs allocated to the Mexico and Canada surrogates are shown in Table 3-24.

Table 3-23. Canadian Spatial Surrogates

Code	Canadian Surrogate Description	Code	Description
100	Population	941	PAVED ROADS
101	total dwelling	942	UNPAVED ROADS
106	ALL_INDUST	945	Commercial Marine Vessels
113	Forestry and logging	950	Combination of Forest and Dwelling
115	Agriculture and forestry activities	955	UNPAVED_ROADS_AND_TRAILS
200	Urban Primary Road Miles	960	TOTBEEF
210	Rural Primary Road Miles	965	TOTBEEF_CD
212	Mining except oil and gas	966	TOTPOUL_CD
220	Urban Secondary Road Miles	967	TOTSWIN_CD
221	Total Mining	968	TOTFERT_CD
222	Utilities	970	TOTPOUL
230	Rural Secondary Road Miles	980	TOTSWIN
240	Total Road Miles	990	TOTFERT
308	Food manufacturing	996	urban_area
321	Wood product manufacturing	1211	Oil and Gas Extraction
323	Printing and related support activities	1212	OilSands
324	Petroleum and coal products manufacturing	1251	OFFR_TOTFERT
326	Plastics and rubber products manufacturing	1252	OFFR_MINES

Code	Canadian Surrogate Description	Code	Description
327	Non-metallic mineral product manufacturing	1253	OFFR Other Construction not Urban
331	Primary Metal Manufacturing	1254	OFFR Commercial Services
412	Petroleum product wholesaler-distributors	1255	OFFR Oil Sands Mines
416	Building material and supplies wholesaler-distributors	1256	OFFR Wood industries CANVEC
448	clothing and clothing accessories stores	1257	OFFR Unpaved Roads Rural
562	Waste management and remediation services	1258	OFFR_Utilities
921	Commercial Fuel Combustion	1259	OFFR total dwelling
923	TOTAL INSTITUTIONAL AND GOVERNEMNT	1260	OFFR_water
924	Primary Industry	1261	OFFR_ALL_INDUST
925	Manufacturing and Assembly	1262	OFFR Oil and Gas Extraction
926	Distribtution and Retail (no petroleum)	1263	OFFR_ALLROADS
927	Commercial Services	1264	OFFR_OTHERJET
931	OTHERJET	1265	OFFR_CANRAIL
932	CANRAIL	--	--

Table 3-24. CAPs Allocated to Mexican and Canadian Spatial Surrogates for 2015, 12US1 domain

Code	Mexican or Canadian Surrogate Description	NH_3	NO_X	PM_{2_5}	SO_2	VOC
11	MEX 2015 Population	26,089	119,206	4,128	473	142,715
14	MEX Residential Heating - Wood	0	1,323	16,963	203	116,625
16	MEX Residential Heating - Distillate Oil	0	13	0	4	0
20	MEX Residential Heating - LP Gas	0	5,649	171	0	96
22	MEX Total Road Miles	2,725	360,388	10,170	5,886	73,886
24	MEX Total Railroads Miles	0	22,751	508	199	887
26	MEX Total Agriculture	177,847	135,558	28,722	6,492	10,886
32	MEX Commercial Land	0	75	1,634	0	23,657
34	MEX Industrial Land	4	1,109	1,975	0	120,470
36	MEX Commercial plus Industrial Land	0	2,123	30	5	98,045
38	MEX Commercial plus Institutional Land	3	1,699	76	3	49
40	MEX Residential (RES1-4)+Comercial+Industrial+Institutional+Government	0	4	11	0	76,212
42	MEX Personal Repair (COM3)	0	0	0	0	5,773
44	MEX Airports Area	0	3,410	97	441	1,166
50	MEX Mobile sources - Border Crossing	5	146	1	3	267
100	CAN Population	734	63	743	13	338

Code	Mexican or Canadian Surrogate Description	NH_3	NO_X	PM_{2_5}	SO_2	VOC
101	CAN total dwelling	407	34,757	2,561	4,641	145,170
106	CAN ALL_INDUST	0	0	11,653	0	72
113	CAN Forestry and logging	470	2,558	0	145	7,191
115	CAN Agriculture and forestry activities	51	610	2,944	13	1,710
200	CAN Urban Primary Road Miles	1,959	94,879	4,176	330	12,707
210	CAN Rural Primary Road Miles	788	57,758	2,318	136	5,511
212	CAN Mining except oil and gas	0	0	3,493	0	0
220	CAN Urban Secondary Road Miles	3,669	144,985	7,901	704	31,364
221	CAN Total Mining	0	0	56,431	0	0
222	CAN Utilities	79	9,604	54,336	3,356	201
230	CAN Rural Secondary Road Miles	2,055	100,286	4,328	361	14,470
240	CAN Total Road Miles	44	80,391	2,918	85	129,307
308	CAN Food manufacturing	0	0	11,188	0	5,908
321	CAN Wood product manufacturing	263	1,801	0	132	7,712
323	CAN Printing and related support activities	0	0	0	0	11,633
324	CAN Petroleum and coal products manufacturing	0	1,023	1,232	391	6,070
326	CAN Plastics and rubber products manufacturing	0	0	0	0	23,640
327	CAN Non-metallic mineral product manufacturing	0	0	6,696	0	0
331	CAN Primary Metal Manufacturing	0	156	5,509	52	74
412	CAN Petroleum product wholesaler-distributors	0	0	0	0	40,256
448	CAN clothing and clothing accessories stores	0	0	0	0	113
562	CAN Waste management and remediation services	220	1,652	2,316	2,282	16,280
921	CAN Commercial Fuel Combustion	192	24,167	2,258	3,890	1,156
923	CAN TOTAL INSTITUTIONAL AND GOVERNEMNT	0	0	0	0	13,910
924	CAN Primary Industry	0	0	0	0	35,614
925	CAN Manufacturing and Assembly	0	0	0	0	70,395
926	CAN Distribtution and Retail (no petroleum)	0	0	0	0	7,096
927	CAN Commercial Services	0	0	0	0	30,629
932	CAN CANRAIL	54	120,110	2,796	433	5,984
941	CAN PAVED ROADS	0	0	303,031	0	0
945	CAN Commercial Marine Vessels	226	185,290	6,730	41,449	15,215
948	CAN Forest	0	0	0	0	0
950	CAN Combination of Forest and Dwelling	1,807	20,074	165,440	2,868	234,530

Code	Mexican or Canadian Surrogate Description	NH_3	NO_X	PM_{2_5}	SO_2	VOC
955	CAN UNPAVED_ROADS_AND_TRAILS	0	0	446,328	0	0
960	CAN TOTBEEF	0	0	1,241	0	264,838
965	CAN TOTBEEF_CD	280,587	0	0	0	0
966	CAN TOTPOUL_CD	23,914	0	0	0	0
967	CAN TOTSWIN_CD	68,007	0	0	0	0
968	CAN TOTFERT_CD	120,175	0	0	0	0
970	CAN TOTPOUL	0	0	182	0	243
980	CAN TOTSWIN	0	0	757	0	2,590
990	CAN TOTFERT	0	4,244	380,084	9,470	155
996	CAN urban_area	0	0	1,275	0	0
1211	CAN Oil and Gas Extraction	2	29	228,601	152	922
1212	CAN OilSands	126	2,053	0	638	1,754
1251	CAN OFFR_TOTFERT	109	118,228	8,760	79	10,875
1252	CAN OFFR_MINES	42	41,668	3,461	31	4,197
1253	CAN OFFR Other Construction not Urban	27	23,675	3,900	20	9,548
1254	CAN OFFR Commercial Services	34	17,872	2,209	29	22,802
1255	CAN OFFR Oil Sands Mines	0	0	0	0	0
1256	CAN OFFR Wood industries CANVEC	14	11,836	1,126	10	1,973
1257	CAN OFFR Unpaved Roads Rural	33	9,929	1,706	29	66,779
1258	CAN OFFR_Utilities	16	8,618	533	14	10,248
1259	CAN OFFR total dwelling	17	5,425	1,415	15	34,693
1260	CAN OFFR_water	9	2,246	334	13	20,148
1261	CAN OFFR_ALL_INDUST	4	4,176	267	3	861
1262	CAN OFFR Oil and Gas Extraction	1	1,061	59	1	151
1263	CAN OFFR_ALLROADS	2	1,087	76	1	507
1264	CAN OFFR_OTHERJET	1	849	71	1	72
1265	CAN OFFR_CANRAIL	0	85	8	0	14

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Appendix A: Nonpoint Oil and Gas (np_oilgas) SCCs

The table below shows the SCCs in the nonpoint oil and gas sector (np_oilgas).

SCC	SCC description
2310000000	Industrial Processes;Oil and Gas Exploration and Production;All Processes;Total: All Processes
2310000220	Industrial Processes;Oil and Gas Exploration and Production;All Processes;Drill Rigs
2310000230	Industrial Processes;Oil and Gas Exploration and Production;All Processes;Workover Rigs
2310000330	Industrial Processes;Oil and Gas Exploration and Production;All Processes;Artificial Lift
2310000550	Industrial Processes;Oil and Gas Exploration and Production;All Processes;Produced Water
2310000660	Industrial Processes;Oil and Gas Exploration and Production;All Processes;Hydraulic Fracturing Engines
2310001000	Industrial Processes;Oil and Gas Exploration and Production;All Processes : On-shore;Total: All Processes
2310002000	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Oil And Gas Production;Total: All Processes
2310002401	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Oil And Gas Production;Pneumatic Pumps: Gas And Oil Wells
2310002411	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Oil And Gas Production;Pressure/Level Controllers
2310002421	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Oil And Gas Production;Cold Vents
2310010000	Industrial Processes;Oil and Gas Exploration and Production;Crude Petroleum;Total: All Processes
2310010100	Industrial Processes;Oil and Gas Exploration and Production;Crude Petroleum;Oil Well Heaters
2310010200	Industrial Processes;Oil and Gas Exploration and Production;Crude Petroleum;Oil Well Tanks - Flashing & Standing/Working/Breathing
2310010300	Industrial Processes;Oil and Gas Exploration and Production;Crude Petroleum;Oil Well Pneumatic Devices
2310010700	Industrial Processes;Oil and Gas Exploration and Production;Crude Petroleum;Oil Well Fugitives
2310010800	Industrial Processes;Oil and Gas Exploration and Production;Crude Petroleum;Oil Well Truck Loading
2310011000	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Oil Production;Total: All Processes
2310011020	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Oil Production;Storage Tanks: Crude Oil
2310011100	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Oil Production;Heater Treater
2310011201	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Oil Production;Tank Truck/Railcar Loading: Crude Oil
2310011500	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Oil Production;Fugitives: All Processes
2310011501	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Oil Production;Fugitives: Connectors
2310011502	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Oil Production;Fugitives: Flanges
2310011503	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Oil Production;Fugitives: Open Ended Lines
2310011504	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Oil Production;Fugitives: Pumps
2310011505	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Oil Production;Fugitives: Valves
2310011506	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Oil Production;Fugitives: Other
2310011600	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Oil Production;Artificial Lift Engines
2310012000	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Oil Production;Total: All Processes
2310012020	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Oil Production;Storage Tanks: Crude Oil
2310012525	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Oil Production;Fugitives, Valves: Oil/Water
2310012526	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Oil Production;Fugitives, Other: Oil/Water
2310020000	Industrial Processes;Oil and Gas Exploration and Production;Natural Gas;Total: All Processes

SCC	SCC description
2310020600	Industrial Processes;Oil and Gas Exploration and Production;Natural Gas;Compressor Engines
2310020700	Industrial Processes;Oil and Gas Exploration and Production;Natural Gas;Gas Well Fugitives
2310020800	Industrial Processes;Oil and Gas Exploration and Production;Natural Gas;Gas Well Truck Loading
2310021010	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Storage Tanks: Condensate
2310021011	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Condensate Tank Flaring
2310021030	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Tank Truck/Railcar Loading: Condensate
2310021100	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Gas Well Heaters
2310021101	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Natural Gas Fired 2Cycle Lean Burn Compressor Engines < 50 HP
2310021102	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Natural Gas Fired 2Cycle Lean Burn Compressor Engines 50 To 499 HP
2310021103	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Natural Gas Fired 2Cycle Lean Burn Compressor Engines 500+ HP
2310021201	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Natural Gas Fired 4Cycle Lean Burn Compressor Engines <50 HP
2310021202	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Natural Gas Fired 4Cycle Lean Burn Compressor Engines 50 To 499 HP
2310021203	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Natural Gas Fired 4Cycle Lean Burn Compressor Engines 500+ HP
2310021251	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Lateral Compressors 4 Cycle Lean Burn
2310021300	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Gas Well Pneumatic Devices
2310021301	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Natural Gas Fired 4Cycle Rich Burn Compressor Engines <50 HP
2310021302	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Natural Gas Fired 4Cycle Rich Burn Compressor Engines 50 To 499 HP
2310021303	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Natural Gas Fired 4Cycle Rich Burn Compressor Engines 500+ HP
2310021310	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Gas Well Pneumatic Pumps
2310021351	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Lateral Compressors 4 Cycle Rich Burn
2310021400	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Gas Well Dehydrators
2310021402	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Nat Gas Fired 4Cycle Rich Burn Compressor Engines 50 To 499 HP w/NSCR
2310021403	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Nat Gas Fired 4Cycle Rich Burn Compressor Engines 500+ HP w/NSCR
2310021411	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Gas Well Dehydrators - Flaring
2310021450	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Wellhead
2310021500	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Gas Well Completion - Flaring
2310021501	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Fugitives: Connectors
2310021502	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Fugitives: Flanges
2310021503	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Fugitives: Open Ended Lines
2310021504	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Fugitives: Pumps
2310021505	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Fugitives: Valves

SCC	SCC description
2310021506	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Fugitives: Other
2310021509	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Fugitives: All Processes
2310021600	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Gas Well Venting
2310021601	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Gas Well Venting - Initial Completions
2310021602	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Gas Well Venting - Recompletions
2310021603	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Gas Well Venting - Blowdowns
2310021604	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Gas Well Venting - Compressor Startups
2310021605	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Gas Well Venting - Compressor Shutdowns
2310021700	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Miscellaneous Engines
2310022000	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Gas Production;Total: All Processes
2310022010	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Gas Production;Storage Tanks: Condensate
2310022051	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Gas Production;Turbines: Natural Gas
2310022090	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Gas Production;Boilers/Heaters: Natural Gas
2310022105	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Gas Production;Diesel Engines
2310022410	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Gas Production;Amine Unit
2310022420	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Gas Production;Dehydrator
2310022506	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Gas Production;Fugitives, Other: Gas
2310023010	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;Storage Tanks: Condensate
2310023030	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;Tank Truck/Railcar Loading: Condensate
2310023100	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;CBM Well Heaters
2310023102	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;CBM Fired 2Cycle Lean Burn Compressor Engines 50 To 499 HP
2310023202	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;CBM Fired 4Cycle Lean Burn Compressor Engines 50 To 499 HP
2310023251	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;Lateral Compressors 4 Cycle Lean Burn
2310023300	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;Pneumatic Devices
2310023302	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;CBM Fired 4Cycle Rich Burn Compressor Engines 50 To 499 HP
2310023310	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;Pneumatic Pumps
2310023351	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;Lateral Compressors 4 Cycle Rich Burn
2310023400	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;Dehydrators
2310023509	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;Fugitives
2310023511	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;Fugitives: Connectors
2310023512	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;Fugitives: Flanges

SCC	SCC description
2310023513	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;Fugitives: Open Ended Lines
2310023515	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;Fugitives: Valves
2310023516	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;Fugitives: Other
2310023600	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;CBM Well Completion: All Processes
2310023603	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;CBM Well Venting - Blowdowns
2310023606	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;Mud Degassing
2310030300	Industrial Processes;Oil and Gas Exploration and Production;Natural Gas Liquids;Gas Well Water Tank Losses
2310030401	Industrial Processes;Oil and Gas Exploration and Production;Natural Gas Liquids;Gas Plant Truck Loading
2310111100	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Oil Exploration;Mud Degassing
2310111401	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Oil Exploration;Oil Well Pneumatic Pumps
2310111700	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Oil Exploration;Oil Well Completion: All Processes
2310112401	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Oil Exploration;Oil Well Pneumatic Pumps
2310121100	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Exploration;Mud Degassing
2310121401	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Exploration;Gas Well Pneumatic Pumps
2310121700	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Exploration;Gas Well Completion: All Processes
2310122100	Industrial Processes;Oil and Gas Exploration and Production;Off-Shore Gas Exploration;Mud Degassing
2310321010	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production - Conventional;Storage Tanks: Condensate
2310321400	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production - Conventional;Gas Well Dehydrators
2310321603	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production - Conventional;Gas Well Venting - Blowdowns
2310400220	Industrial Processes;Oil and Gas Exploration and Production;All Processes - Unconventional;Drill Rigs
2310421010	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production - Unconventional;Storage Tanks: Condensate
2310421100	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production - Unconventional;Gas Well Heaters
2310421400	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production - Unconventional;Gas Well Dehydrators
2310421603	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production - Unconventional;Gas Well Venting - Blowdowns

Appendix B: **Profiles (other than onroad) that are new or revised in SPECIATE4.5 that were used in the 2015 platform**

Sector	Pollutant	Profile code	Profile description	SPECIATE version	comment
nonpt	VOC	G95223TOG	Poultry Production - Average of Production Cycle with gapfilled methane and ethane	5.0 (not yet released)	Replacement for v4.5 profile 95223; Used 70% methane, 20% ethane, and the 10% remaining VOC is from profile 95223
Nonpt, ptnonipm	VOC	G95240TOG	Beef Cattle Farm and Animal Waste with gapfilled methane and ethane	5.0 (not yet released)	Replacement for v4.5 profile 95240. Used 70% methane, 20% ethane; the 10% remaining VOC is from profile 95240.
nonpt	VOC	G95241TOG	Swine Farm and Animal Waste	5.0 (not yet released)	Replacement for v4.5 profile 95241. Used 70% methane, 20% ethane; the 10% remaining VOC is from profile 95241
nonpt, ptnonipm, pt_oilgas, ptegu	PM2.5	95475	Composite -Refinery Fuel Gas and Natural Gas Combustion	5.0 (not yet released)	Composite of AE6-ready versions of SPECIATE4.5 profies 95125, 95126, and 95127
nonroad	VOC	95328	Spark-Ignition Exhaust Emissions from 2-stroke off-road engines - E10 ethanol gasoline	4.5	
nonroad	VOC	95330	Spark-Ignition Exhaust Emissions from 4-stroke off-road engines - E10 ethanol gasoline	4.5	
nonroad	VOC	95331	Diesel Exhaust Emissions from Pre-Tier 1 Off-road Engines	4.5	
nonroad	VOC	95332	Diesel Exhaust Emissions from Tier 1 Off-road Engines	4.5	
nonroad	VOC	95333	Diesel Exhaust Emissions from Tier 2 Off-road Engines	4.5	
np_oilgas	VOC	95087a	Oil and Gas - Composite - Oil Field - Oil Tank Battery Vent Gas	4.5	
np_oilgas	VOC	95109a	Oil and Gas - Composite - Oil Field - Condensate Tank Battery Vent Gas	4.5	
np_oilgas	VOC	95398	Composite Profile - Oil and Natural Gas Production - Condensate Tanks	4.5	
np_oilgas	VOC	95403	Composite Profile - Gas Wells	4.5	
np_oilgas	VOC	95417	Oil and Gas Production - Composite Profile - Untreated Natural Gas, Uinta Basin	4.5	
np_oilgas	VOC	95418	Oil and Gas Production - Composite Profile - Condensate Tank Vent Gas, Uinta Basin	4.5	
np_oilgas	VOC	95419	Oil and Gas Production - Composite Profile - Oil Tank Vent Gas, Uinta Basin	4.5	
np_oilgas	VOC	95420	Oil and Gas Production - Composite Profile - Glycol Dehydrator, Uinta Basin	4.5	

np_oilgas	VOC	DJVNT_R	Oil and Gas -Denver-Julesburg Basin Produced Gas Composition from Non-CBM Gas Wells	4.5	
np_oilgas	VOC	FLR99	Natural Gas Flare Profile with DRE >98%	4.5	
np_oilgas	VOC	PNC01_R	Oil and Gas -Piceance Basin Produced Gas Composition from Non-CBM Gas Wells	4.5	
np_oilgas	VOC	PNC02_R	Oil and Gas -Piceance Basin Produced Gas Composition from Oil Wells	4.5	
np_oilgas	VOC	PNC03_R	Oil and Gas -Piceance Basin Flash Gas Composition for Condensate Tank	4.5	
np_oilgas	VOC	PNCDH	Oil and Gas Production - Composite Profile - Glycol Dehydrator, Piceance Basin	4.5	
np_oilgas	VOC	PRBCB_R	Oil and Gas -Powder River Basin Produced Gas Composition from CBM Wells	4.5	
np_oilgas	VOC	PRBCO_R	Oil and Gas -Powder River Basin Produced Gas Composition from Non-CBM Wells	4.5	
np_oilgas	VOC	PRM01_R	Oil and Gas -Permian Basin Produced Gas Composition for Non-CBM Wells	4.5	
np_oilgas	VOC	SSJCB_R	Oil and Gas -South San Juan Basin Produced Gas Composition from CBM Wells	4.5	
np_oilgas	VOC	SSJCO_R	Oil and Gas -South San Juan Basin Produced Gas Composition from Non-CBM Gas Wells	4.5	
np_oilgas	VOC	SWFLA_R	Oil and Gas -SW Wyoming Basin Flash Gas Composition for Condensate Tanks	4.5	
np_oilgas	VOC	SWVNT_R	Oil and Gas -SW Wyoming Basin Produced Gas Composition from Non-CBM Wells	4.5	
np_oilgas	VOC	UNT01_R	Oil and Gas -Uinta Basin Produced Gas Composition from CBM Wells	4.5	
np_oilgas	VOC	WRBCO_R	Oil and Gas -Wind River Basin Produced Gas Composition from Non-CBM Gas Wells	4.5	
pt_oilgas	VOC	95325	Chemical Manufacturing Industry Wide Composite	4.5	
pt_oilgas	VOC	95326	Pulp and Paper Industry Wide Composite	4.5	
pt_oilgas, ptnonipm	VOC	95399	Composite Profile - Oil Field - Wells	4.5	
pt_oilgas	VOC	95403	Composite Profile - Gas Wells	4.5	
pt_oilgas	VOC	95417	Oil and Gas Production - Composite Profile - Untreated Natural Gas, Uinta Basin	4.5	
pt_oilgas	VOC	DJVNT_R	Oil and Gas -Denver-Julesburg Basin Produced Gas Composition from Non-CBM Gas Wells	4.5	
pt_oilgas, ptnonipm	VOC	FLR99	Natural Gas Flare Profile with DRE >98%	4.5	
pt_oilgas	VOC	PNC01_R	Oil and Gas -Piceance Basin Produced Gas Composition from Non-CBM Gas Wells	4.5	
pt_oilgas	VOC	PNC02_R	Oil and Gas -Piceance Basin Produced Gas Composition from Oil Wells	4.5	
pt_oilgas	VOC	PNCDH	Oil and Gas Production - Composite Profile - Glycol Dehydrator, Piceance Basin	4.5	
pt_oilgas, ptnonipm	VOC	PRBCO_R	Oil and Gas -Powder River Basin Produced Gas Composition from Non-CBM Wells	4.5	

pt_oilgas, ptnoniom	VOC	PRM01_R	Oil and Gas -Permian Basin Produced Gas Composition for Non-CBM Wells	4.5	
pt_oilgas, ptnonipm	VOC	SSJCO_R	Oil and Gas -South San Juan Basin Produced Gas Composition from Non-CBM Gas Wells	4.5	
pt_oilgas, ptnonipm	VOC	SWVNT_R	Oil and Gas -SW Wyoming Basin Produced Gas Composition from Non-CBM Wells	4.5	
ptfire	VOC	95421	Composite Profile - Prescribed fire southeast conifer forest	4.5	
ptfire	VOC	95422	Composite Profile - Prescribed fire southwest conifer forest	4.5	
ptfire	VOC	95423	Composite Profile - Prescribed fire northwest conifer forest	4.5	
ptfire	VOC	95424	Composite Profile - Wildfire northwest conifer forest	4.5	
ptfire	VOC	95425	Composite Profile - Wildfire boreal forest	4.5	
ptnonipm	VOC	95325	Chemical Manufacturing Industry Wide Composite	4.5	
ptnonipm	VOC	95326	Pulp and Paper Industry Wide Composite	4.5	
onroad	PM2.5	95462	Composite - Brake Wear	4.5	Used in SMOKE-MOVES
onroad	PM2.5	95460	Composite - Tire Dust	4.5	Used in SMOKE-MOVES

Appendix C: CB6 Assignment for New Species

RAMBOLL ENVIRON

September 27, 2016

MEMORANDUM

To: Alison Eyth and Madeleine Strum, OAQPS, EPA
From: Ross Beardsley and Greg Yarwood, Ramboll Environ
Subject: Species Mappings for CB6 and CB05 for use with SPECIATE 4.5

Summary

Ramboll Environ (RE) reviewed version 4.5 of the SPECIATE database, and created CB05 and CB6 mechanism species mappings for newly added compounds. In addition, the mapping guidelines for Carbon Bond (CB) mechanisms were expanded to promote consistency in current and future work.

Background

The Environmental Protection Agency's SPECIATE repository contains gas and particulate matter speciation profiles of air pollution sources, which are used in the generation of emissions data for air quality models (AQM) such as CMAQ (http://www.cmascenter.org/cmaq/) and CAMx (http://www.camx.com). However, the condensed chemical mechanisms used within these photochemical models utilize fewer species than SPECIATE to represent gas phase chemistry, and thus the SPECIATE compounds must be assigned to the AQM model species of the condensed mechanisms. A chemical mapping is used to show the representation of organic chemical species by the model compounds of the condensed mechanisms.

This memorandum describes how chemical mappings were developed from SPECIATE 4.5 compounds to model species of the CB mechanism, specifically CB05 (http://www.camx.com/publ/pdfs/CB05_Final_Report_120805.pdf) and CB6 (http://aqrp.ceer.utexas.edu/projectinfoFY12_13/12-012/12-012%20Final%20Report.pdf).

Methods

CB Model Species

Organic gases are mapped to the CB mechanism either as explicitly represented individual compounds (e.g. ALD2 for acetaldehyde), or as a combination of model species that represent common structural groups (e.g. ALDX for other aldehydes, PAR for alkyl groups). Table 1 lists all of the explicit and structural model species in CB05 and CB6 mechanisms, each of which represents a defined number of carbon atoms allowing for carbon to be conserved in all cases. CB6 contains four more explicit model species than CB05 and an additional structural group to represent ketones. The CB05 representation of the five additional CB6 species is provided in the '*Included in CB05*' column of Table 1.

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UNC-EMAQ(4-02)-16

In addition to the explicit and structural species, there are two model species that are used to represent organic gases that are not treated by the CB mechanism:

NVOL – Very low volatility SPECIATE compounds that reside predominantly in the particle phase and should be excluded from the gas phase mechanism. These compounds are mapped by setting NVOL equal to the molecular weight (e.g. decabromodiphenyl oxide is mapped as 959.2 NVOL), which allows for the total mass of all NVOL to be determined.

UNK – Compounds that are unable to be mapped to CB using the available model species. This approach should be avoided unless absolutely necessary, and will lead to a warning message in the speciation tool.

Table 1. Model species in the CB05 and CB6 chemical mechanisms.

Model Species Name	Description	Number of Carbons	Included in CB05 (structural mapping)	Included in CB6
Explicit model species				
ACET	Acetone (propanone)	3	No (3 PAR)	Yes
ALD2	Acetaldehyde (ethanal)	2	Yes	Yes
BENZ	Benzene	6	No (1 PAR, 5 UNR)	Yes
CH4	Methane	1	Yes	Yes
ETH	Ethene (ethylene)	2	Yes	Yes
ETHA	Ethane	2	Yes	Yes
ETHY	Ethyne (acetylene)	2	No (1 PAR, 1 UNR)	Yes
ETOH	Ethanol	2	Yes	Yes
FORM	Formaldehyde (methanal)	1	Yes	Yes
ISOP	Isoprene (2-methyl-1,3-butadiene)	5	Yes	Yes
MEOH	Methanol	1	Yes	Yes
PRPA	Propane	3	No (1.5 PAR, 1.5 UNR)	Yes
Common Structural groups				
ALDX	Higher aldehyde group (-C-CHO)	2	Yes	Yes
IOLE	Internal olefin group (R_1R_2>C=C<R_3R_4)	4	Yes	Yes
KET	Ketone group (R_1R_2 >C=O)	1	No (1 PAR)	Yes
OLE	Terminal olefin group (R_1R_2>C=C)	2	Yes	Yes
PAR	Paraffinic group (R_1-C<R_2R_3)	1	Yes	Yes
TERP	Monoterpenes	10	Yes	Yes
TOL	Toluene and other monoalkyl aromatics	7	Yes	Yes
UNR	Unreactive carbon groups (e.g., halogenated carbons)	1	Yes	Yes
XYL	Xylene and other polyalkyl aromatics	8	Yes	Yes
Not mapped to CB model species				
NVOL	Very low volatility compounds	*	Yes	Yes
UNK	Unknown	*	Yes	Yes

*Each NVOL represents 1 g mol^{-1} and low volatility compounds are assigned to NVOL based on molecular weight. UNK is unmapped and thus does not represent any carbon.

Mapping guidelines for non-explicit organic gases using CB model species

SPECIATE compounds that are not treated explicitly are mapped to CB model species that represent common structural groups. Table 2 lists the carbon number and general mapping guidelines for each of the structure model species.

Table 2. General Guidelines for mapping using CB6 structural model species.

CB6 Species Name	Number of Carbons	Represents
ALDX	2	Aldehyde group. ALDX represents 2 carbons and additional carbons are represented as alkyl groups (mostly PAR), e.g. propionaldehyde is ALDX + PAR
IOLE	4	Internal olefin group. IOLE represents 4 carbons and additional carbons are represented as alkyl groups (mostly PAR), e.g. 2-pentene isomers are IOLE + PAR. *Exceptions:* • IOLE with 2 carbon branches on both sides of the double bond are downgraded to OLE
KET	1	Ketone group. KET represents 1 carbon and additional carbons are represented as alkyl groups (mostly PAR), e.g. butanone is 3 PAR + KET
OLE	2	Terminal olefin group. OLE represents 2 carbons and additional carbons are represented as alkyl groups (mostly PAR), e.g. propene is OLE + PAR. Alkyne group, e.g. butyne isomers are OLE + 2 PAR.
PAR	1	Alkanes and alkyl groups. PAR represents 1 carbon, e.g. butane is 4 PAR. See UNR for exceptions.
TERP	10	All monoterpenes are represented as 1 TERP.
TOL	7	Toluene and other monoalkyl aromatics. TOL represents 7 carbons and any additional carbons are represented as alkyl groups (mostly PAR), e.g. ethylbenzene is TOL + PAR. Cresols are represented as TOL and PAR. Styrenes are represented using TOL, OLE and PAR.
UNR	1	Unreactive carbons are 1 UNR such as quaternary alkyl groups (e.g., neo-pentane is 4 PAR + UNR), carboxylic acid groups (e.g., acetic acid is PAR + UNR), ester groups (e.g., methyl acetate is 2 PAR + UNR), halogenated carbons (e.g., trichloroethane isomers are 2 UNR), carbons of nitrile groups (-C≡N).
XYL	8	Xylene isomers and other polyalkyl aromatics. XYL represents 8 carbons and any additional carbons are represented as alkyl groups (mostly PAR), e.g. trimethylbenzene isomers are XYL + PAR

Some compounds that are multifunctional and/or include hetero-atoms lack obvious CB mappings. We developed guidelines for some of these compound classes to promote consistent representation in this work and future revisions. Approaches for several compound classes are explained in Table 3. We developed guidelines as needed to address newly added species in SPECIATE 4.5 but did not systematically review existing mappings for "difficult to assign" compounds that could benefit from developing a guideline.

Table 3. Mapping guidelines for some difficult to map compound classes and structural groups

Compound Class/Structural group	CB model species representation
Chlorobenzenes and other halogenated benzenes	Guideline: • 3 or less halogens – 1 PAR, 5 UNR • 4 or more halogens – 6 UNR Examples: • 1,3,5-Chlorobenzene – 1 PAR, 5 UNR • Tetrachlorobenzenes – 6 UNR
Cyclodienes	Guideline: • 1 IOLE with additional carbons represented as alkyl groups (generally PAR) Examples: • Methylcyclopentadiene – 1 IOLE, 2 PAR • Methylcyclohexadiene – 1 IOLE, 3 PAR
Furans/Pyrroles	Guideline: • 2 OLE with additional carbons represented as alkyl groups (generally PAR) Examples: • 2-Butylfuran – 2 OLE, 4 PAR • 2-Pentylfuran – 2 OLE, 5 PAR • Pyrrole – 2 OLE • 1-Methylpyrrole – 2 OLE, 1 PAR
Heterocyclic aromatic compounds containing 2 non-carbon atoms	Guideline: • 1 OLE with remaining carbons represented as alkyl groups (generally PAR) Examples: • Ethylpyrazine – 1 OLE, 4 PAR • 1-methylpyrazole – 1 OLE, 2 PAR • 4,5-Dimethyloxazole – 1 OLE, 3 PAR
Triple bond(s)	Guideline: • Triple bonds are treated as PAR unless they are the only reactive functional group. If a compound contains more than one triple bond and no other reactive functional groups, then one of the triple bonds is treated as OLE with additional carbons treated as alkyl groups. Examples: • 1-Penten-3-yne – 1 OLE, 3 PAR • 1,5-Hexadien-3-yne – 2 OLE, 2 PAR • 1,6-Heptadiyne – 1 OLE, 5 PAR

These guidelines were used to map the new species from SPEICATE4.5, and also to revise some previously mapped compounds. Overall, a total of 175 new species from SPECIATEv4.5 were mapped and 7 previously mapped species were revised based on the new guidelines.

Recommendation

1. Complete a systematic review of the mapping of all species to ensure conformity with current mapping guidelines. The assignments of existing compounds that are similar to new species were reviewed and revised to promote consistency in mapping approaches, but the majority of existing species mappings were not reviewed as it was outside the scope of this work.
2. Develop a methodology for classifying and tracking larger organic compounds based on their volatility (semi, intermediate, or low volatility) to improve support for secondary organic aerosol (SOA) modeling using the volatility basis set (VBS) SOA model, which is available in both CMAQ and CAMx. A preliminary investigation of the possibility of doing so has been performed, and is discussed in a separate memorandum.