

Technical Support Document (TSD)
Preparation of Emissions Inventories for the Version 7.1
2016 North American Emissions Modeling Platform

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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
BPS	Bulk Plant Storage
BTP	Bulk Terminal (Plant) to Pump
C1C2	Category 1 and 2 commercial marine vessels
C3	Category 3 (commercial marine vessels)
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
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

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
ICI	Industrial/Commercial/Institutional (boilers and process heaters)
ICR	Information Collection Request
I/M	Inspection and Maintenance
IMO	International Marine Organization
IPM	Integrated Planning Model
ITN	Itinerant
LADCO	Lake Michigan Air Directors Consortium
LDGHG	Light-Duty Vehicle Greenhouse Gas
LPG	Liquified 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
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
NH₃	Ammonia
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
PFC	Portable Fuel Container
PM_{2.5}	Particulate matter less than or equal to 2.5 microns
PM₁₀	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
SESARM	Southeastern States Air Resource Managers
SESQ	Sesquiterpenes
SMARTFIRE	Satellite Mapping Automated Reanalysis Tool for Fire Incident Reconciliation
SMOKE	Sparse Matrix Operator Kernel Emissions
SO₂	Sulfur dioxide
SOA	Secondary Organic Aerosol
SIP	State Implementation Plan
SPDPRO	Hourly Speed Profiles for weekday versus weekend
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), working in conjunction with the National Emissions Inventory Collaborative, developed an air quality modeling platform for air toxics and criteria air pollutants that represents the year 2016 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 2016 “alpha” 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 2016 for some emissions sectors.

This 2016 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 National Emissions Inventory Collaborative is a partnership between state emissions inventory staff, multi-jurisdictional organizations (MJOs), federal land managers (FLMs), EPA, and others to develop a North American air pollution emissions modeling platform with a base year of 2016 for use in air quality planning. The Collaborative planned for three versions of the 2016 platform: alpha, beta, and Version 1.0. The version of the platform described in this document is the “2016 alpha platform”, although this study incorporated additional fixes and updates that were not part of the original 2016 alpha platform that was released in March, 2018. The 2016 alpha platform was used to support air quality modeling applications using CMAQ version 5.2 and CAMx version 6.5. 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 (NO_x) 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. The CAMx model uses a similar, but slightly different, chemical mechanism, as described in Section 2.1.

The 2016 alpha platform consists of one ‘complete’ emissions case: the 2016 base case, i.e., 2016fe_16j. This platform accounts for atmospheric chemistry and transport within a state of the art photochemical grid model. In the case abbreviation 2016fe_16j, 2016 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”); where the “e” stands for the fifth set of emissions modeled for a 2014-based modeling platform.

The emissions data in the 2016 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 represented 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 2016.

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://www.smoke-model.org/>), 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 2016 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 (GHRSSST) (see <https://www.ghrsst.org/>) and is given the EPA meteorological case label “16j.” The full case name includes this abbreviation following the emissions portion of the case name to fully specify the name of the case as “2016fe_16j.”

This document contains five sections and several appendices. Section 2 describes the 2016 inventories input to SMOKE. Section 3 describes the emissions modeling and the ancillary files used with the emission inventories. Data summaries are provided in Section 4. Section 5 provides references. The Appendices provide additional details about specific technical methods or data.

2 2016 Emission Inventories and Approaches

This section describes the 2016 emissions data that make up the 2016 alpha 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 2016, and other adjustments made to support modeling as described here. Documentation for the 2014NEIv2, including a TSD, is available at <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.

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 2016 platform.

Compared to the 2014v7.1 emissions modeling platform, which is based directly on the 2014NEIv2, the 2016v7.1 alpha emissions modeling platform includes emissions for the year 2016 for some data categories. The point source emission inventories for platform include partially updated emissions for 2016. Agricultural and wildland fire emissions represent the year 2016. 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, SO₂ emissions were updated to reflect new rules on sulfur emissions that took effect in the year 2015. For fertilizer ammonia emissions, a 2016-specific emissions inventory is used in this platform. Area source oil and gas emissions were projected from 2014NEIv2 to better represent 2016.

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. Onroad emissions for the 2016 alpha platform were developed based on emissions factors output from MOVES2014a for the year 2016 run with inputs derived from the 2014NEIv2 including activity data projected to the year 2016. MOVES2014a replaced the National Mobile Inventory Model (NMIM) as the interface for using the NONROAD2008 model, thus 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.

For the purposes of preparing the air quality model-ready emissions, the NEI was split into finer-grained sectors used for emissions modeling. 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.

Table 2-1 presents the sectors in the 2016 platform 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.

Table 2-1. Platform sectors for the 2016v7.1 (alpha) emissions modeling platform

Platform Sector: <i>abbreviation</i>	NEI Data Category	Description and resolution of the data input to SMOKE
EGU units: <i>ptegu</i>	Point	Point source EGUs for 2016 from the Emissions Inventory System (EIS), based on 2014NEIv2 with some sources updated to 2016. The inventory emissions are replaced with hourly 2016 Continuous Emissions Monitoring System (CEMS) values for NO _x and SO ₂ for any units that are matched to the NEI, and other pollutants for matched units are scaled from the 2016 point inventory using CEMS heat input. Emissions for all sources not matched to CEMS data come from the raw inventory. Annual resolution for sources not matched to CEMS data, hourly for CEMS sources.
Point source oil and gas: <i>pt_oilgas</i>	Point	Point sources for 2016 that include oil and gas production and related processes based on facilities with the following NAICS: 2111, 21111, 211111, 211112 (Oil and Gas Extraction); 213111 (Drilling Oil and Gas Wells); 213112 (Support Activities for Oil and Gas Operations); 2212, 22121, 221210 (Natural Gas Distribution); 48611, 486110 (Pipeline Transportation of Crude Oil); 4862, 48621, 486210 (Pipeline Transportation of Natural Gas). Includes offshore oil and gas platforms in the Gulf of Mexico (FIPs=85). Oil and gas point sources that were not already updated to 2016 in the baseline inventory were projected from 2014 to 2016. Annual resolution.
Remaining non-EGU point: <i>ptnonipm</i>	Point	All 2016 point source records not matched to the <i>ptegu</i> or <i>pt_oilgas</i> sectors. Includes all aircraft and airport ground support emissions and some rail yard emissions. Annual resolution.
Agricultural: <i>ag</i>	Nonpoint	Nonpoint livestock and fertilizer application emissions. Livestock includes ammonia and other pollutants (except PM _{2.5}) and is from 2014NEIv2. Fertilizer includes only ammonia and is estimated for 2016 using the FEST-C model. County and monthly resolution.
Agricultural fires with point resolution: <i>ptagfire</i>	Nonpoint	2016 agricultural fire sources that were developed by EPA as point sources with day-specific emissions. They are in the nonpoint NEI data category, but in the platform, they are treated as point sources.
Area fugitive dust: <i>afdust</i>	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 NEI emissions are reduced during modeling according to a transport fraction and a meteorology-based (precipitation and snow/ice cover) zero-out. County and annual resolution.
Biogenic: <i>beis</i>	Nonpoint	Year 2016, hour-specific, grid cell-specific emissions generated from the BEIS3.61 model within SMOKE, including emissions in Canada and Mexico using BELD v4.1 land use data (slightly updated from the BELDv4.1 used in 2014v7.0).
Category 1, 2 CMV: <i>cmv_c1c2</i>	Nonpoint	Category 1 (C1) and category 2 (C2) commercial marine vessel (cmv) emissions sources from the 2014NEIv2 nonpoint inventory, except that it does not use emissions from the 2014 NEI in Federal Waters. For 2016 modeling, SO ₂ emissions are reduced by 90% compared to 2014NEIv2. County and annual resolution.

Platform Sector: <i>abbreviation</i>	NEI Data Category	Description and resolution of the data input to SMOKE
Category 3 CMV: <i>cmv_c3</i>	Nonpoint	Category 3 (C3) cmv emissions converted to point sources based on the center of the grid cells. Includes C3 emissions in U.S. state and Federal waters, and also all non-U.S. C3 emissions except those in Canadian waters. For 2016 modeling, SO ₂ emissions are reduced by 90% compared to 2014NEIv2.
locomotives: <i>rail</i>	Nonpoint	Rail locomotives emissions from the 2014NEIv2. County and annual resolution.
Remaining nonpoint: <i>nonpt</i>	Nonpoint	2014NEIv2 nonpoint sources not included in other platform sectors. County and annual resolution.
Nonpoint source oil and gas: <i>np_oilgas</i>	Nonpoint	2014NEIv2 nonpoint sources from oil and gas-related processes, projected to 2016. County and annual resolution.
Residential Wood Combustion: <i>rwc</i>	Nonpoint	2014NEIv2 nonpoint sources from residential wood combustion (RWC) processes. County and annual resolution.
Nonroad: <i>nonroad</i>	Nonroad	2016 nonroad equipment emissions developed with the MOVES2014a using NONROAD2008 version NR08a and new HAP emission factors than had been used in the 2011NEI and 2014NEIv2. MOVES was used for all states except California, which submitted their own emissions. County and monthly resolution.
Onroad: <i>onroad</i>	Onroad	2016 onroad mobile source gasoline and diesel vehicles from moving and non-moving vehicles that drive on roads, along with vehicle refueling. 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 emissions tables produced by MOVES2014a.
Onroad California: <i>onroad_ca_adj</i>	Onroad	2016 California-provided CAP onroad mobile source gasoline and diesel vehicles submitted to the NEI, gridded and temporalized using MOVES2014a. Volatile organic compound (VOC) HAP emissions derived from California-provided VOC emissions and MOVES-based speciation.
Point source fires- <i>ptfire</i>	Events	Point source day-specific wildfires and prescribed fires for 2016 computed using SMARTFIRE2 for both flaming and smoldering processes (i.e., SCCs 281XXXX002). Smoldering is forced into layer 1 (by adjusting heat flux).
Non-US. fires: <i>ptfire_othna</i>	N/A	Point source day-specific wildfires and prescribed fires for 2016 provided by Environment Canada with data for missing months, and for Mexico and Central America, filled in using fires from the Fire INventory (FINN) from National Center for Atmospheric Research (NCAR) fires (NCAR, 2016 and Wiedinmyer, C., 2011).
Other dust sources not from the 2014 NEI: <i>othafdust</i>	N/A	Fugitive dust sources from Canada's 2013 and 2025 inventories (interpolated to 2016). A transport fraction adjustment is applied along with a meteorology-based (precipitation and snow/ice cover) zero-out. Also includes afdust emissions in Alaska, Hawaii, Puerto Rico, and Virgin Islands from 2014NEIv2. County and annual resolution.
Other point sources not from the 2014 NEI: <i>othpt</i>	N/A	Point sources from Canada's 2013 and 2025 inventories (interpolated to 2016) and for Mexico 2014 and 2018 inventories projected from their 2008 inventory and then interpolated to 2016, annual resolution.

Platform Sector: <i>abbreviation</i>	NEI Data Category	Description and resolution of the data input to SMOKE
Other non-NEI nonpoint and nonroad: <i>othar</i>	N/A	Year 2016 Canada (province or sub-province resolution) emissions, interpolated from 2013 and 2025: monthly for agricultural ammonia and nonroad sources; annual for rail, CMV and other nonpoint Canada sectors. Year 2016 Mexico (municipio resolution), interpolated between year 2014 and 2018 projections from their 2008 inventory: annual nonpoint and nonroad mobile inventories.
Other non-NEI onroad sources: <i>onroad_can</i>	N/A	Monthly year 2016 Canada (province resolution or sub-province resolution, depending on the province) onroad mobile inventory, interpolated from 2013 and 2025. Also includes onroad emissions in Alaska, Hawaii, Puerto Rico, and Virgin Islands from 2014NEIv2.
Other non-NEI onroad sources: <i>onroad_mex</i>	N/A	Monthly year 2016 Mexico (municipio resolution) onroad mobile inventory, interpolated from 2014 and 2018 inventories developed with MOVES-Mexico.

The emission inventories in SMOKE input formats for the 2016 alpha platform are available from the EPA’s Air Emissions Modeling website for the alpha platform: <https://www.epa.gov/air-emissions-modeling/2014-2016-version-7-air-emissions-modeling-platforms>, under the section entitled “2016v7.1 (alpha) Platform” The 2016 alpha platform “README” file indicates the particular zipped files associated with each platform sector. A number of reports (i.e., summaries) are available with the data files for the 2016 platform. The types of reports include state summaries of inventory pollutants and model species by modeling platform sector and county annual totals by modeling platform sector.

The remainder of Section 2 provides details about the data contained in each of the 2016 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 2016 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). 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.

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. Point inventories are also available in EIS for interim years such as 2016. In this interim point inventory, larger sources are updated with emissions for year 2016, 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 2016 into the Flat File 2010 (FF10) format that is compatible with SMOKE (<https://www.emascenter.org/smoke/documentation/4.5/html/ch08s02s08.html>). For the 2016 alpha platform, the export of point source emissions from EIS, including stack parameters and locations, was performed on March 27, 2018. At that time, EIS did not include a complete set of emissions for

hydrochloric acid (HCL) or chlorine (CL2) for 2016, which are needed for CMAQ modeling. These pollutants typically are augmented within EIS for sources which do not already have them. Augmentation of HCL and CL2 had only been partially performed within EIS at that time and had not yet incorporated the Toxics Release Inventory (TRI) dataset, which includes HCL and CL2 emissions by facility for 2016. For facilities where HCL and CL2 emissions in the 2016 inventory were greater than or equal to the emissions reported in the TRI dataset, inferring that the HCL and CL2 emissions in the 2016 inventory were already complete, no additional changes were made to the inventory. For sources where the TRI emissions were greater than the EIS emissions, HCL and CL2 emissions were added to the inventory for those facilities, using stack parameters, source coordinates, and other point source identifiers from the 2014NEIv2 point inventory where possible. HCL and CL2 records in the 2016 point inventory that were augmented based on the TRI dataset are indicated with data_set_id = "HCL_CL2_Augment_TRI". The only other major differences between the 2016 point inventory exported from EIS and the inventory used for modeling involve identification of additional EGUs and matching CEMs for the ptegu sector, and removal of EGUs for which there are no CEMS NOx emissions in 2016.

As in the 2014v7.0 and 2014v7.1 platforms, all changes to release parameters that would occur in SMOKE as a result of missing values or values outside SMOKE internally set ranges in the FF10 file prior to SMOKE run were incorporated. This was done for two reasons: 1) to provide better transparency in the FF10 files with respect to the data used in the model, and 2) to ensure that emission inputs are consistent across CMAQ and AERMOD models since both use the FF10 as the starting point. Because SMOKE uses metric units (i.e., m and K) for defaults, these are converted to the English units (ft and F) as specified by the FF10 file format. Out-of-range criteria were changed from v7.0 to be consistent with the EIS quality assurance checks (as opposed to the default ranges in SMOKE). Other than velocities, for which the EIS range for flowrate and velocity were inconsistent, no parameters in the NEI had to be changed due to not falling within the EIS range. Out of range values existed because the flow range checks in EIS allow some velocities to be above or below the range and we ran the velocity check after computing the missing flowrates.

Table 2-2 through Table 2-4 show conditions for which changes are made to the NEI values in the modeling file. The "Records changed" column indicates how many records were changed in the 2014NEIv2 version of the point file and provide the keywords used in the FF10 that indicate that a release parameter was changed and the situation. Table 2-5 describes the comment incorporated into the SMOKE made for each change. Even though SMOKE does not use the fugitive release point parameters for CMAQ, they are included in the table for completeness.

Table 2-2. Release parameter changes to the SMOKE Modeling flat file for point sources-For point sources with stack releases (ERPtype NOT equal to "1")

Field	Existing value	New value	Conditions/notes	Records changed
Stkhgt	missing	Use SMOKE defaults		None
Stkdiam	missing	Use SMOKE defaults		None

Field	Existing value	New value	Conditions/notes	Records changed
Stkvel	missing	calculate from stkflow and stkdiam if not missing; otherwise use SMOKE defaults	vel = $4 * \text{stkflow} / (\pi * \text{stkdiam}^2)$ If the flow and diam are missing such that you cannot compute, then use new value based pstk or global defaults.	1,473,185 No pstk values used <i>ERPVelCompute</i>
Stktemp	missing	Use SMOKE defaults		None
Stkhgt	Outside EIS range	use minimum value or maximum value in feet	Less than 1 ft (0.3048 m) or greater than 1300 ft (396 m)	None
Stkdiam	Outside EIS range	use minimum value or maximum value in ft	Less than 0.001 ft (0.0003048 m) or greater than 300 ft (91.4 m)	None
Stkvel	Outside EIS range	use minimum value or maximum value in ft/s	Less than 0.001ft/s (0.0003048 m/s) or greater than 1000 ft/s (304.8 m/s)	Below min: 18,817 Above max: 11,742 <i>ERPVelRange</i>
stktemp	Outside SMOKE tolerance	use minimum value or maximum value in F	Less than -30 F (-34.4 C or 248.15 K) or greater than 4000 F (2204.4 C or 2477.6 K)	None

Table 2-3. Release parameter changes to the SMOKE Modeling flat file for point sources-For Fugitive Release Points

Field	Existing value	New value	Conditions/notes	Records changed
fug_width_ydim	missing	32.808 ft		3,856,867; <i>ERPFugMissing</i>
fug_length_xdim	missing	32.808 ft		3,888,847; <i>ERPFugMissing</i>
fug_angle	missing	0		3,932,478; <i>ERPFugMissing</i>
fug_height	missing	10 ft	fug_width_ydim and fug_length_xdim are missing	3,556,330; <i>ERPFugMissing</i>
fug_height	missing	0	WHEN fug_width_ydim and fug_length_xdim are not missing and > 0	12,742 <i>ERPFugHeight0</i>

Table 2-4. Release parameter changes to the SMOKE Modeling flat file for point sources-For Coke Ovens, any release point that emits coke oven emissions (pollutant code 140)

Field	Existing value	New value	Conditions/notes	Records changed
stkhgt	< 126 ft	126 ft	erptype NOT = "1"	2159; <i>ERPCokeoven126</i>
fug_height	< 126 ft	126 ft	erptype = "1"	2829; <i>ERPCokeoven126</i>
fug_length_xdim	< 50 ft	50 ft	erptype = "1"	2767; <i>ERPCokeovenFug50</i>
fug_width_ydim	< 50 ft	50 ft	erptype = "1"	2767; <i>ERPCokeovenFug50</i>

Table 2-5. Description of Comments added to SMOKE Modeling flat file used when defaulting or changing values from the NEI

Comment	Description
<i>ERPHtRange</i>	height in the inventory was out of range
<i>ERPDiamRange</i>	diameter in the inventory was out of range
<i>ERPVelRange</i>	velocity in the inventory or velocity calculated from the flowrate in the inventory was out of range
<i>ERPTempRange</i>	Temperature in the inventory was out of range
<i>ERPFugMissing</i>	fugitive height, length and width are missing or fugitive length and/or width are missing
<i>ERPFugHeight0</i>	fugitive height in the inventory was set to 0 because the width and length were not missing
<i>ERPCokeoven126</i>	fugitive or stack height of release point emitting coke oven emissions was less than 126 ft
<i>ERPCokeovenFug50</i>	fugitive length or width was less than 50 ft.

After incorporating the above changes, the flat file was modified to remove sources without specific locations (i.e., their FIPS code ends in 777). Then 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).

The inventory pollutants processed through SMOKE for all point source sectors were: carbon monoxide (CO), NO_x, VOC, sulfur dioxide (SO₂), ammonia (NH₃), particles less than 10 microns in diameter (PM₁₀), and particles less than 2.5 microns in diameter (PM_{2.5}), hydrochloric acid (HCl), and chlorine (Cl₂). The NBAFM species are explicit in the CB6-CMAQ chemical mechanism, but for point sources in the 2016 alpha platform, 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.

The ptnonipm and pt_oilgas sector emissions were provided to SMOKE as annual emissions. For those ptegu sources with CEMS data that could be matched to the 2016 inventory, hourly CEMS NO_x and SO₂ emissions were used rather than the annual total NEI emissions. For all other pollutants at matched units, the annual emissions were used as-is from the NEI, but, were allocated to hourly values using heat input from the CEMS data. For the sources in the ptegu sector not matched to CEMS data, daily emissions were created using an approach described in Section 2.1.1. For non-CEMS units other than municipal waste combustors and cogeneration units, IPM region- and pollutant-specific diurnal profiles were applied to create hourly emissions.

2.1.1 EGU sector (ptegu)

The ptegu sector contains emissions from EGUs in the 2016 alpha 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 2016 CEMS data from EPA's Clean Air Markets Division (CAMD) via ORIS facility codes and boiler ID. For the matched units, SMOKE replaces the 2016 emissions of NO_x and SO₂ 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 (except those changed as discussed in Table 2-2). 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 NO_x 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, pollutant², 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

² The year to day profiles use NO_x and SO₂ CEMS for NO_x and SO₂, respectively. For all other pollutants, they use heat input CEMS data.

IPM region. See Section 3.5.2 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 2-6. 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 2-6. 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
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 2016, and sources with emissions carried forward from 2014NEIv2 with no updates. For this study, sources already updated for the year 2016 in EIS were used as-is. The emissions carried forward from 2014NEIv2 were projected to 2016. Projection factors for 2016 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 2-7, 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 2016 pt_oilgas inventory used for this study consists of both sources already updated to 2016 within EIS (used directly), and sources carried forward from 2014NEIv2 (projected to 2016).

Table 2-7. Oil and gas sector 2016 projection factors

State	Oil projection factor	Gas projection factor	Average projection factor
Alabama	0.825	0.910	0.868
Alaska	0.989	1.019	1.004
Arizona	0.143	0.443	0.293
Arkansas	1.125	0.733	0.929

State	Oil projection factor	Gas projection factor	Average projection factor
California	0.909	0.858	0.883
Colorado	1.214	1.035	1.125
Florida	0.868	1.080	0.974
Illinois	0.905	1.132	1.018
Indiana	0.725	0.938	0.831
Kansas	0.769	0.850	0.809
Kentucky	0.769	0.984	0.876
Louisiana	0.821	0.890	0.855
Maryland	1.000	1.700	1.700
Michigan	0.758	0.874	0.816
Mississippi	0.837	0.891	0.864
Missouri	0.628	0.333	0.480
Montana	0.776	0.881	0.828
Nebraska	0.740	1.273	1.007
Nevada	0.877	1.000	0.938
New Mexico	1.171	1.014	1.093
New York	0.624	0.666	0.645
North Dakota	0.958	1.314	1.136
Ohio	1.475	2.810	2.142
Oklahoma	1.055	1.059	1.057
Oregon	1.000	0.820	0.820
Pennsylvania	0.921	1.248	1.085
South Dakota	0.783	0.661	0.722
Tennessee	0.779	0.681	0.730
Texas	1.018	0.939	0.979
Utah	0.746	0.802	0.774
Virginia	0.500	0.900	0.700
West Virginia	0.987	1.289	1.138
Wyoming	0.953	0.925	0.939

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 2016-specific emissions, while emissions for smaller sources that were not submitted for the 2016 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 2016 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 in 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-tds>, 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 2016 modeling platform sectors, along with any data that were replaced with non-NEI data or projected for 2016.

2.2.1 Area fugitive dust sector (afdust)

The area-source fugitive dust (afdust) sector contains PM₁₀ 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., PM₁₀ and PM_{2.5}) considered to be “fugitive” dust sources. These SCCs are provided in Table 2-8. Table 2-9 shows the SCCs that would have also been included in this sector if they had emissions in the 2014 NEI.

Table 2-8. SCCs in the afdust platform sector from NEI2014v2: nonzero emissions

SCC	SCC Description
2294000000	Mobile Sources;Paved Roads;All Paved Roads;Total: Fugitives

SCC	SCC Description
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
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

SCC	SCC Description
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 2-9. SCCs in the afdust platform sector from 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 to 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 2016 alpha platform uses the same unadjusted afdust emissions inventory as the 2014v7.1 platform, except that meteorological adjustments are based on 2016 meteorology instead of 2014 meteorology.

The total impacts of the transport fraction and meteorological adjustments are shown in Table 2-10 after backing out the meteorological adjustment applied in the 2014NEIv2. The amount of the reduction ranges from about 94 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 2016 would look slightly different depending on the meteorology for each year, but the general pattern would be the same.

Table 2-10. Total impact of 2016 fugitive dust adjustments to unadjusted 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	531,293	62,937	-438,671	-51,997	83%	83%

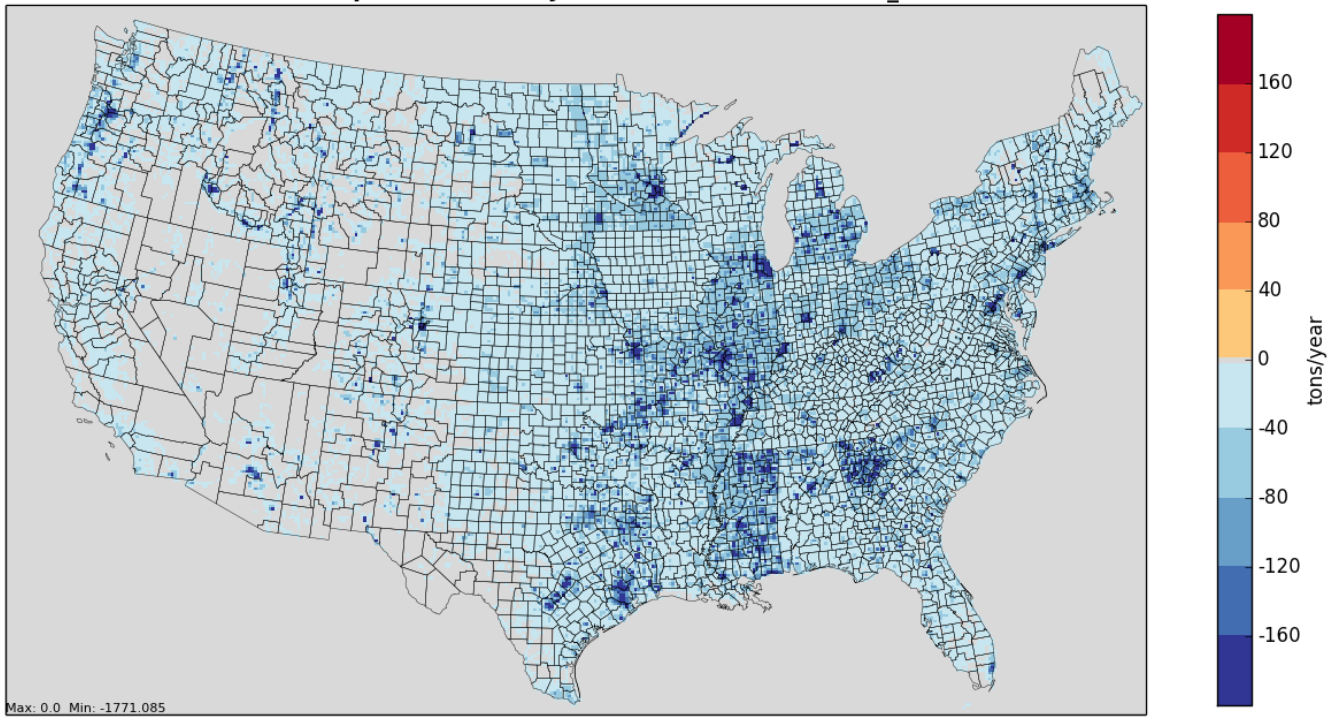
State	Unadjusted * PM₁₀	Unadjusted * PM_{2.5}	Change in PM₁₀	Change in PM_{2.5}	PM₁₀ Reduction	PM_{2.5} Reduction
Arizona	263,125	32,553	-87,885	-10,853	33%	33%
Arkansas	319,496	49,010	-228,479	-34,266	71%	70%
California	312,634	41,077	-144,062	-18,498	46%	45%
Colorado	240,391	36,454	-139,202	-20,316	58%	55%
Connecticut	23,464	3,341	-20,583	-2,936	88%	88%
Delaware	14,316	2,456	-10,454	-1,800	73%	73%
District of Columbia	2,547	367	-1,932	-277	75%	75%
Florida	715,494	81,268	-445,103	-50,357	63%	62%
Georgia	552,231	65,601	-458,075	-54,088	83%	83%
Idaho	449,835	55,636	-299,519	-36,055	67%	65%
Illinois	994,307	143,485	-647,183	-93,160	65%	64%
Indiana	713,793	83,925	-531,386	-62,342	75%	74%
Iowa	384,852	59,826	-241,936	-37,560	63%	62%
Kansas	610,450	98,980	-295,548	-46,914	48%	47%
Kentucky	311,270	42,672	-244,594	-33,289	79%	78%
Louisiana	265,757	35,626	-191,357	-25,271	72%	71%
Maine	37,846	5,854	-34,175	-5,310	90%	91%
Maryland	103,136	16,220	-80,553	-12,624	77%	77%
Massachusetts	147,627	18,236	-127,438	-15,662	87%	86%
Michigan	388,603	48,408	-307,739	-38,155	79%	79%
Minnesota	403,260	61,397	-296,519	-44,688	73%	72%
Mississippi	432,583	53,230	-350,713	-42,515	81%	80%
Missouri	1,597,370	184,016	-1,170,745	-134,315	74%	73%
Montana	431,167	61,792	-275,027	-37,722	64%	61%
Nebraska	347,803	55,013	-176,311	-27,704	51%	50%
Nevada	159,216	22,770	-37,590	-5,235	23%	23%
New Hampshire	21,762	4,476	-20,281	-4,169	94%	94%
New Jersey	39,910	9,017	-31,436	-7,082	79%	79%
New Mexico	487,322	53,646	-169,159	-18,644	35%	35%
New York	266,587	44,926	-225,543	-38,051	85%	85%
North Carolina	201,723	29,163	-166,360	-24,065	82%	82%
North Dakota	472,269	82,353	-285,360	-49,598	60%	60%
Ohio	926,270	115,558	-714,546	-88,754	77%	77%
Oklahoma	448,827	67,546	-234,212	-34,417	52%	51%
Oregon	656,174	73,388	-510,850	-55,666	78%	76%
Pennsylvania	239,408	37,266	-204,741	-31,915	85%	85%
Rhode Island	4,773	759	-3,723	-592	78%	78%

State	Unadjusted * PM ₁₀	Unadjusted * PM _{2.5}	Change in PM ₁₀	Change in PM _{2.5}	PM ₁₀ Reduction	PM _{2.5} Reduction
South Carolina	161,909	21,449	-126,440	-16,760	78%	78%
South Dakota	337,913	62,999	-192,859	-35,808	57%	56%
Tennessee	292,101	42,813	-236,307	-34,482	81%	80%
Texas	1,253,345	178,124	-639,339	-88,138	51%	49%
Utah	207,734	26,019	-111,731	-13,796	54%	53%
Vermont	22,131	3,212	-20,038	-2,898	91%	90%
Virginia	283,722	36,631	-239,744	-30,957	85%	85%
Washington	239,794	41,136	-140,928	-24,047	59%	58%
West Virginia	122,180	15,017	-112,762	-13,862	92%	92%
Wisconsin	687,613	89,370	-532,980	-68,885	78%	77%
Wyoming	239,512	29,074	-131,571	-15,750	55%	54%
Domain Total	18,366,850	2,486,092	-12,333,687	-1,642,242	67%	66%

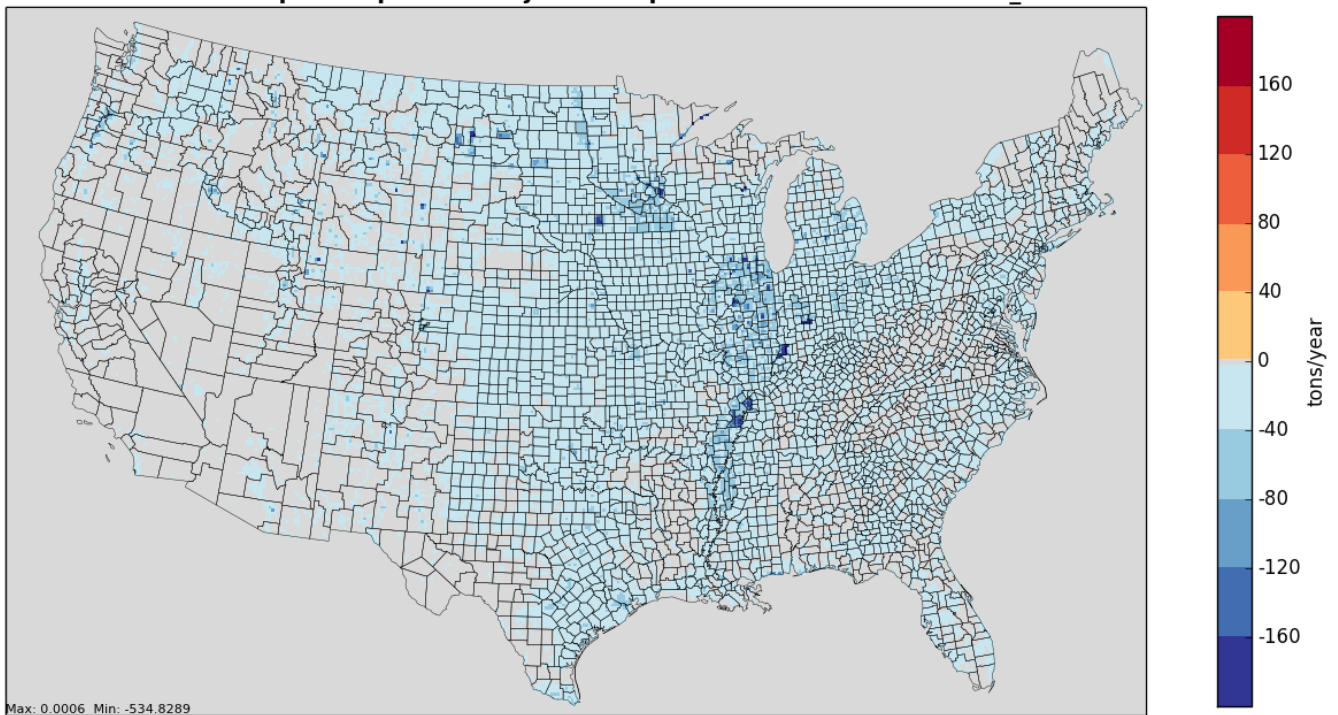
* Unadjusted" here does not mean raw 2014NEIv2, it means 2014NEIv2 with met adjustments backed out as appropriate (i.e. the inventory that was fed into SMOKE)

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

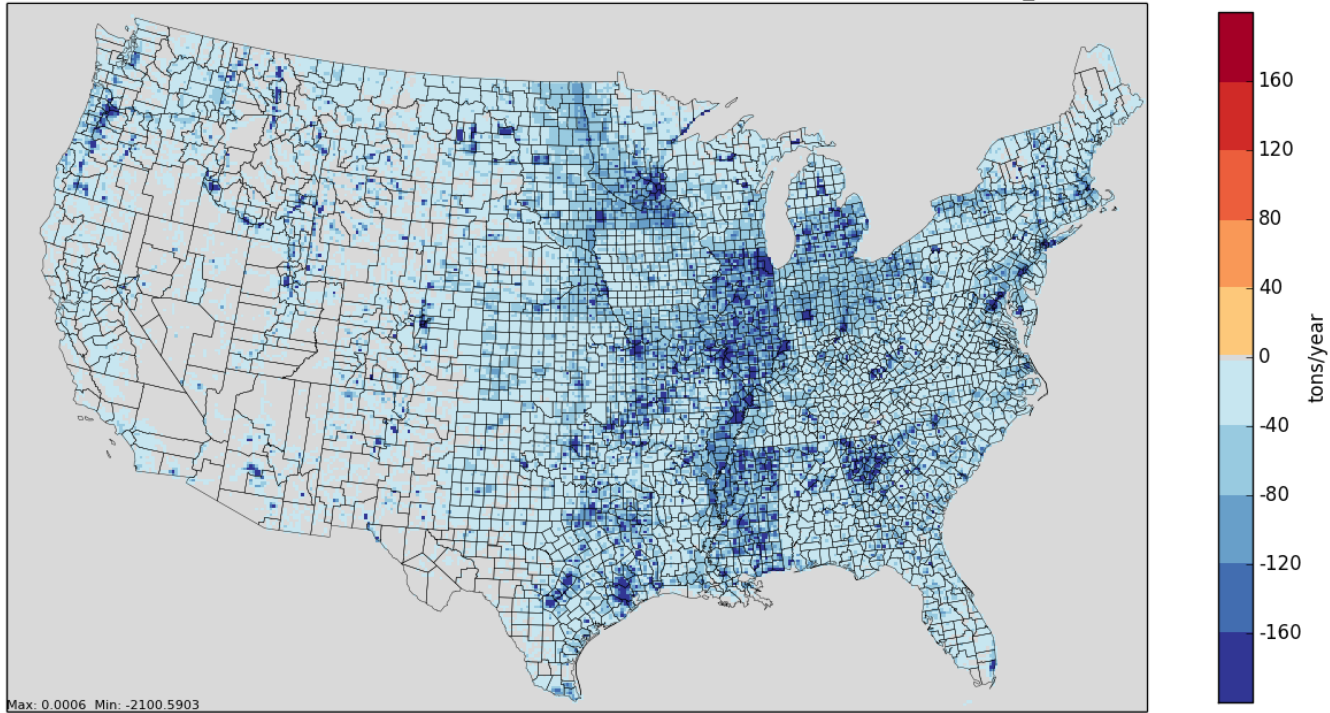
2014fa Xportfrac - Unadjusted Annual Afdust PM2_5



2014fa Precip and Xportfrac Adjusted - Xportfrac Annual Afdust PM2_5



2014fa Precip and Xportfrac Adjusted - Unadjusted Annual Afdust PM2_5



2.2.2 Agricultural sector (ag)

The “ag” sector includes NH₃ emissions from fertilizer from 2016, 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 shown in Table 2-11 and 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.

The fertilizer SCCs are shown in Table 2-12 and consist of 15 specific types of ammonia-based fertilizer and one for miscellaneous fertilizers. The “ag” sector includes all of the NH₃ emissions from fertilizer from the NEI. However, the “ag” sector does not include all of the livestock NH₃ emissions, as there is a very small amount of NH₃ emissions from livestock in the ptonipm 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 NH₃, 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 2-11. Livestock SCCs extracted from the NEI to create the ag sector

SCC	SCC Description*	NH ₃ + 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	

SCC	SCC Description*	NH3+ other pollutants
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 2-12. 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

SCC	SCC Description*
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

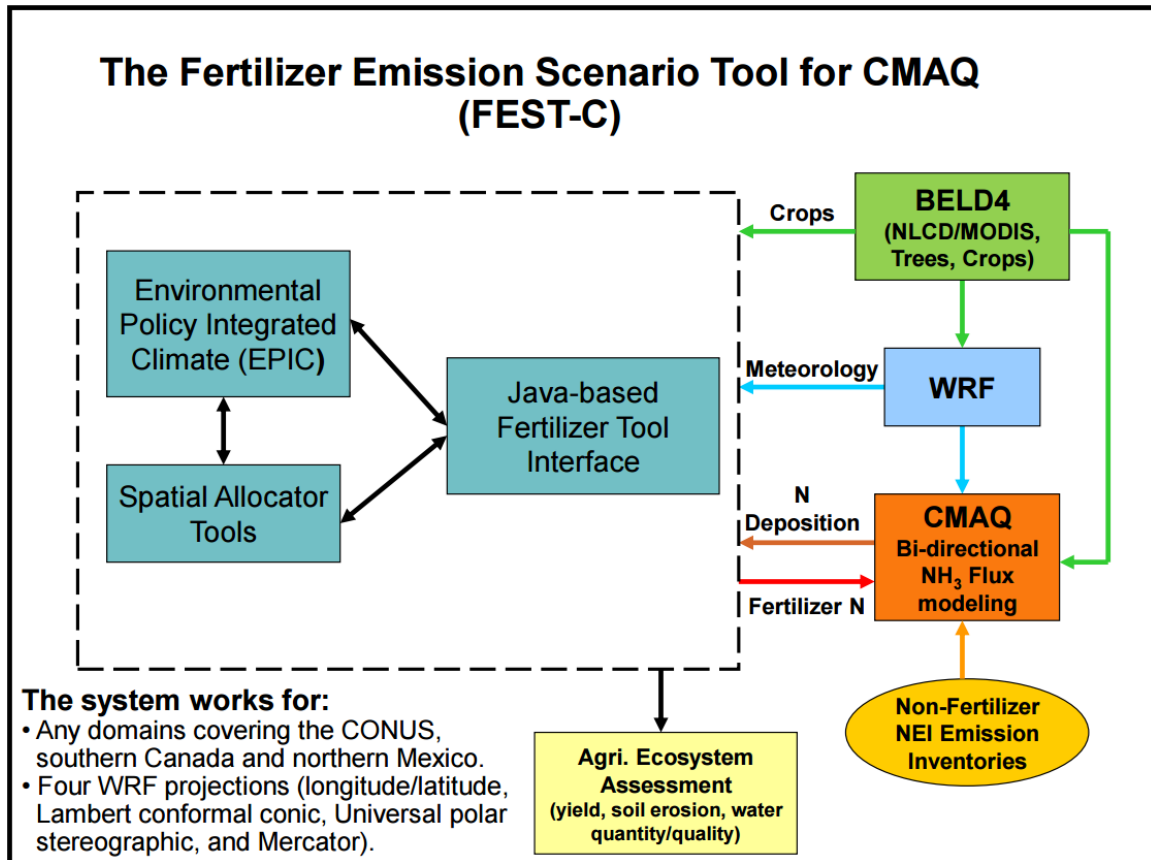
* All descriptions include “Miscellaneous Area Sources; Agriculture Production – Crops; Fertilizer Application” as the beginning of the description.

Fertilizer emissions for 2016 are based on the FEST-C model. The bidirectional version of CMAQ (v5.3) and the Fertilizer Emissions Scenario Tool for CMAQ FEST-C (v1.3) were used to estimate ammonia (NH₃) emissions from agricultural soils. The approach to estimate 2016 fertilizer emissions consists of these steps:

- Run FEST-C and CMAQ model with bidirectional (“bidi”) NH₃ exchange to produce nitrate (NO₃), Ammonium (NH₄⁺, including Urea), and organic (manure) nitrogen (N) fertilizer usage estimates, and gaseous ammonia NH₃ emission estimates respectively.
- Calculate county-level emission factors as the ratio of bidirectional CMAQ NH₃ fertilizer emissions to FEST-C total N fertilizer application.
- Assign the NH₃ emissions to one SCC: “...Miscellaneous Fertilizers” (2801700099).

The Fertilizer Emission Scenario Tool for CMAQ (FEST-C) is the software program that processes land use and agricultural activity data to develop inputs for the CMAQ model when run with bidirectional exchange. FEST-C reads land use data from the Biogenic Emissions Landuse Dataset (BELD), meteorological variables from the Weather Research and Forecasting model, and nitrogen deposition data from a previous or historical average CMAQ simulation. FEST-C, then uses the USDA’s Environmental Policy Integrated Climate (EPIC) modeling system to simulate the agricultural practices and soil biogeochemistry and provides information regarding fertilizer timing, composition, application method and amount.

Figure 2-2. “Bidi” modeling system used to compute 2016 Fertilizer Application emissions



The following activity parameters were input into the EPIC model:

- Grid cell meteorological variables from WRF (see Table 3)
- Initial soil profiles/soil selection
- Presence of 21 major crops: irrigated and rain fed hay, alfalfa, grass, barley, beans, grain corn, silage corn, cotton, oats, peanuts, potatoes, rice, rye, grain sorghum, silage sorghum, soybeans, spring wheat, winter wheat, canola, and other crops (e.g. lettuce, tomatoes, etc.)
- Fertilizer sales to establish the type/composition of nutrients applied
- Management scenarios for the 10 USDA production regions. These include irrigation, tile drainage, intervals between forage harvest, fertilizer application method (injected versus surface applied), and equipment commonly used in these production regions.

We used the WRF meteorological model to provide grid cell meteorological parameters for 2016 using a national 12-km rectangular grid covering the continental U.S. The meteorological parameters in Table 2-13 were used as EPIC model inputs.

Table 2-13. Environment variables needed for an EPIC simulation

EPIC input variable	Variable Source
Daily Total Radiation (MJ m ²)	WRF
Daily Maximum 2-m Temperature (C)	WRF

EPIC input variable	Variable Source
Daily minimum 2-m temperature (C)	WRF
Daily Total Precipitation (mm)	WRF
Daily Average Relative Humidity (unitless)	WRF
Daily Average 10-m Wind Speed (m s⁻¹)	WRF
Daily Total Wet Deposition Oxidized N (g/ha)	CMAQ
Daily Total Wet Deposition Reduced N (g/ha)	CMAQ
Daily Total Dry Deposition Oxidized N (g/ha)	CMAQ
Daily Total Dry Deposition Reduced N (g/ha)	CMAQ
Daily Total Wet Deposition Organic N (g/ha)	CMAQ

Initial soil nutrient and pH conditions in EPIC are based on the 1992 USDA Soil Conservation Service (CSC) Soils-5 survey. The EPIC model then is run for 25 years using current fertilization and agricultural cropping techniques to estimate soil nutrient content and pH for the 2016 EPIC/WRF/CMAQ simulation.

The presence of crops in each model grid cell was determined through the use of USDA Census of Agriculture data (2012) and USGS National Land Cover data (2011). These two data sources were used to compute the fraction of agricultural land in a model grid cell and the mix of crops grown on that land.

Fertilizer sales data and the 6-month period in which they were sold were extracted from the 2014 Association of American Plant Food Control Officials (AAPFCO). AAPFCO data are used to identify the composition (e.g. urea, nitrate, organic) of the fertilizer used, and the amount applied is estimated using the modeled crop demand. These data are useful in making a reasonable assignment of what kind of fertilizer is being applied to which crops.

Management activity data refers to data used to estimate representative crop management schemes. We used the USDA Agricultural Resource Management Survey (ARMS) to provide management activity data. These data cover 10 USDA production regions and provide management schemes for irrigated and rain fed hay, alfalfa, grass, barley, beans, grain corn, silage corn, cotton, oats, peanuts, potatoes, rice, rye, grain sorghum, silage sorghum, soybeans, spring wheat, winter wheat, canola, and other crops (e.g. lettuce, tomatoes, etc.).

The emission factors were derived from the 2016 CMAQ FST-C outputs. Total fertilizer emission factors for each month and county were computed by taking the ratio of total fertilizer NH₃ emissions (short tons) to total nitrogen fertilizer application (short tons). 12 km by 12 km gridded NH₃ emissions were mapped to a county shape file polygon. The cell was assigned to a county if the grid centroid fell within the county boundary.

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 3.5.5) 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 2016, 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 2016 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 2016 for this study. The methodology and projection factors for np_oilgas projections were the same as for pt_oilgas, except that 2016 projections were applied to the entire 2014NEIv2 np_oilgas inventory. Projection factors for 2016 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 2-7, 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 2-14.

Residential wood combustion emissions for the 2016 alpha 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 2-14. 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 3.5.4. For the 2016 alpha platform, day-of-year

temporalization is based on 2016 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.

For the 2016 alpha platform, the emissions inventory for the nonpt sector is from 2014NEIv2 and is the same as in the 2014v7.1 platform.

2.3 2016 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 2016 alpha platform includes emission factors processed by MOVES for the year 2016, and projections of

2014NEIv2 vehicle miles traveled, vehicle population, and hoteling (extended idling) hours activity data to 2016.

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 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 2016 alpha 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 2-15.

Table 2-15. 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 2016. The activity data was projected from 2014 to 2016 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/2016/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 Transportation³. VMT projection factors for all states are in Table 2-16.

Table 2-16. Factors applied to project VMT from 2014 to 2016

State	Rural roads	Urban roads
Alabama	5.36%	5.47%
Alaska	8.27%	8.27%
Arizona	1.07%	6.35%
Arkansas	4.80%	5.36%
California	1.06%	2.39%
Colorado	5.97%	6.67%
Connecticut	1.33%	1.45%
Delaware	4.42%	6.75%
District of Columbia	0.00%	2.68%
Florida	10.27%	6.64%
Georgia	10.10%	10.10%
Hawaii	6.14%	4.21%
Idaho	5.51%	7.80%
Illinois	3.40%	1.96%
Indiana	5.02%	5.02%
Iowa	6.17%	6.05%
Kansas	2.42%	6.52%
Kentucky	2.52%	3.26%
Louisiana	-5.49%	7.10%
Maine	3.75%	3.75%
Maryland	4.98%	4.75%
Massachusetts	7.42%	7.42%
Michigan	5.62%	0.66%
Minnesota	2.66%	2.97%
Mississippi	1.83%	4.96%
Missouri	4.70%	4.17%
Montana	3.32%	4.34%
Nebraska	5.54%	5.54%
Nevada	8.30%	5.30%
New Hampshire	5.00%	3.65%
New Jersey	5.41%	2.83%

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
New Mexico	10.01%	10.01%
New York	-4.90%	-4.90%
North Carolina	7.47%	8.41%
North Dakota	-7.35%	-7.35%
Ohio	4.61%	5.42%
Oklahoma	4.72%	1.23%
Oregon	8.05%	4.84%
Pennsylvania	-4.30%	4.73%
Rhode Island	3.26%	3.26%
South Carolina	9.70%	8.89%
South Dakota	3.23%	2.64%
Tennessee	6.29%	6.29%
Texas	7.82%	7.82%
Utah	11.62%	11.62%
Vermont	5.55%	2.24%
Virginia	-4.93%	9.78%
Washington	6.86%	4.43%
West Virginia	2.21%	2.21%
Wisconsin	4.15%	9.32%
Wyoming	-1.38%	-1.53%
Puerto Rico	0.00%	0.00%
Virgin Islands	0.00%	0.00%

Once the VMT dataset was finalized for 2016, VPOP activity for 2016 was calculated by applying VMT/VPOP ratios based on 2014NEIv2 to the projected 2016 VMT for each county, fuel, and vehicle type. Hoteling hours activity for 2016 was calculated in a similar manner, by applying 2014NEIv2-based VMT/hoteling ratios to the projected 2016 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 counties⁴. For these counties, the EPA zeroed out the onroad estimates of refueling (i.e., SCCs =220xxxx62) 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 2016 alpha 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

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.

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 2016 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 2016 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 estimates⁵. 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 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

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, NO₂, HONO and used the PM_{2.5} ratio for PEC, PNO₃, POC, PSO₄, 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.)

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 2016 alpha platform, cmv_c1c2 emissions from the 2014NEIv2 were used as-is, with the exception of SO₂ emissions, which were reduced by 90% from 2014NEIv2 levels in accordance with ECA-IMO emissions standards for 2016. However, it should be noted that this reduction was not appropriate for C1 and C2 ships, because those ships use diesel fuel and not residual fuel; however, since SO₂ emissions levels for C1 and C2 ships are small in 2014NEIv2, this further reduction had a small impact.

Table 2-17 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 2-17. 2014NEI 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 2016 alpha 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 2-18 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 2-18. 2014NEI 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 2016 alpha platform C3 emissions are from 2014NEIv2 within U.S. state and federal waters (FIPS = 85). SO₂ 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.

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.

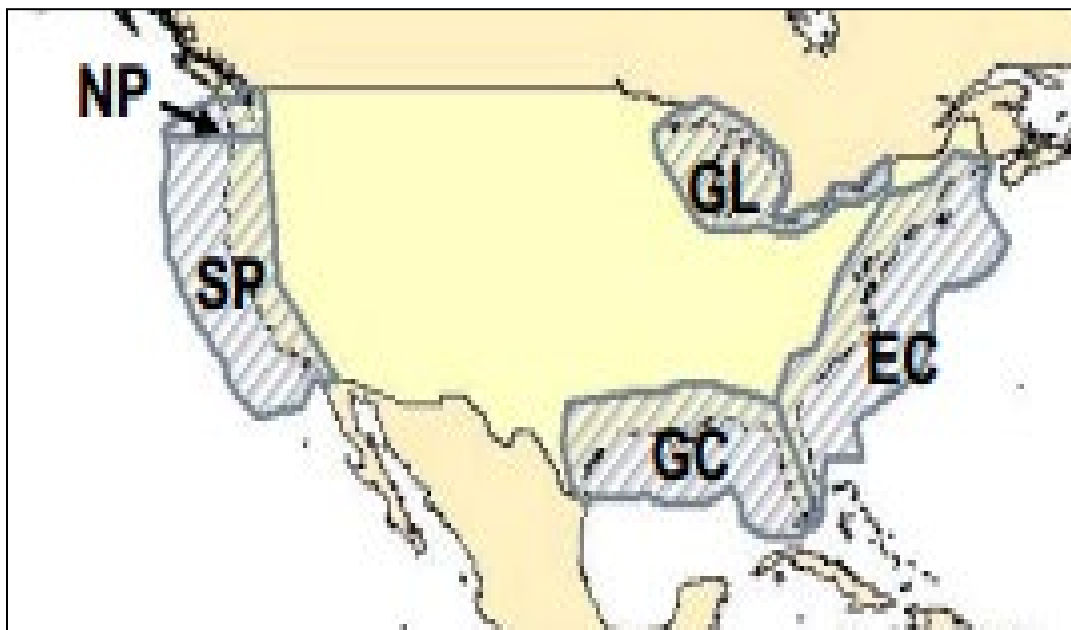
The EPA-“ECA-IMO-based” emissions were developed based on a 4-km resolution ASCII raster format dataset that preserves shipping lanes. This dataset has been used since the ECA-IMO project began in 2005, although it was then known as the Sulfur Emissions Control Area (SECA). The ECA-IMO emissions consist 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, SO₂, 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: PM₁₀, PM_{2.5}, CO, CO₂, NH₃, NO_x, SO_x (assumed to be SO₂), 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 2-19. The geographic regions listed in the table are shown in Figure 2-3. 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 2-19. 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 2-3. 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 2-18.

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 3.2.1.3 for more details on C3 speciation in the cmv sector and Section 3.5.8 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 2-20. 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 2016 alpha platform are from 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. 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 2-20. SCCs used for the 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. A separate MOVES2014a run was performed for the year 2016 and is the basis for nonroad emissions in the 2016 alpha platform. This study includes a corrected nonroad inventory which represents year 2016 emissions. This corrected inventory was developed in May 2018, two months after the 2016 alpha platform was originally published.

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 2016 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 2016 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 2016 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 2016 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 unspciated 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 (othafdust)

For Canadian area and nonroad sources, year-2013 and year-2025 emissions provided by Environment Canada were interpolated to year 2016, including CMV emissions for most pollutants. SO₂ emissions from CMV were set to 2025 values for 2016 modeling, because 2025 SO₂ CMV emissions in Canada more accurately reflect 2016 marine sulfur emissions rules than do emissions from a 2013-to-2025 interpolation. For all pollutants other than SO₂, CMV emissions were interpolated from 2013 and 2025 to 2016. 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.

The 2016 alpha platform includes modeling for the 36US3 domain (see Section 3.4), which includes a portion of Southeast Alaska. The U.S. afdust emissions for 36US3 are based on the 12US1 onroad emissions, and thus do not include Southeast Alaska. Therefore, we include the 2014NEIv2 afdust Alaska emissions inventory when processing the othafdust sector for 36US3. So for 36US3 only, the othafdust sector includes emissions in both Canada and part of Alaska.

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 2016 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 and year-2025 emissions provided by Environment Canada were interpolated to year 2016. 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 2016 for this platform.

The 2016 alpha platform includes modeling for the 36US3 domain (see Section 3.4), which includes a portion of Southeast Alaska. The U.S. onroad emissions for 36US3 are based on the 12US1 onroad emissions, and thus do not include Southeast Alaska. Therefore, we include the 2014NEIv2 onroad Alaska emissions inventory when processing the onroad_can sector for 36US3. So for 36US3 only, the onroad_can sector includes emissions in both Canada and part of Alaska.

2.5.4 Fires from Canada and Mexico (*ptfire_othna*)

Annual 2016 wildland emissions for Mexico, Canada, Central America, and Caribbean nations in the 2016 alpha 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*)

In the 2016 alpha platform, wildfires and prescribed burning emissions are contained in the *ptfire* sector which contain emissions from flaming and smoldering combustion phases. Fire emissions are specified at geographic coordinates (point locations) and have daily emissions values.

The point source day-specific emission estimates for 2016 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 2016 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 for 2016 contain CAPs only, and so the BAFM HAP emissions were obtained using VOC speciation profiles (i.e., a “no-integrate noHAP” use case).

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 2-21.

Table 2-21. 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.”

2.7 Biogenic sources (beis)

Biogenic emissions were developed using the Biogenic Emission Inventory System version 3.61 (BEIS3.61) within SMOKE using the “16j” version of 2016 meteorology. The 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 the 2016 alpha 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 2016 alpha 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 2-22.

Table 2-22. 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/>).

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 2-4, Figure 2-5, Figure 2-6, and Figure 2-7, respectively. The land use changes made in 2014v7.1 and alpha platform would not impact these v7.0-based figures. Biogenic emissions for 2016 are different from 2014 in terms of temporalization and magnitude but, are similar spatially.

Figure 2-4. Annual NO emissions output from BEIS 3.61 for 2014

2014fa_nata beis NO emissions, annual

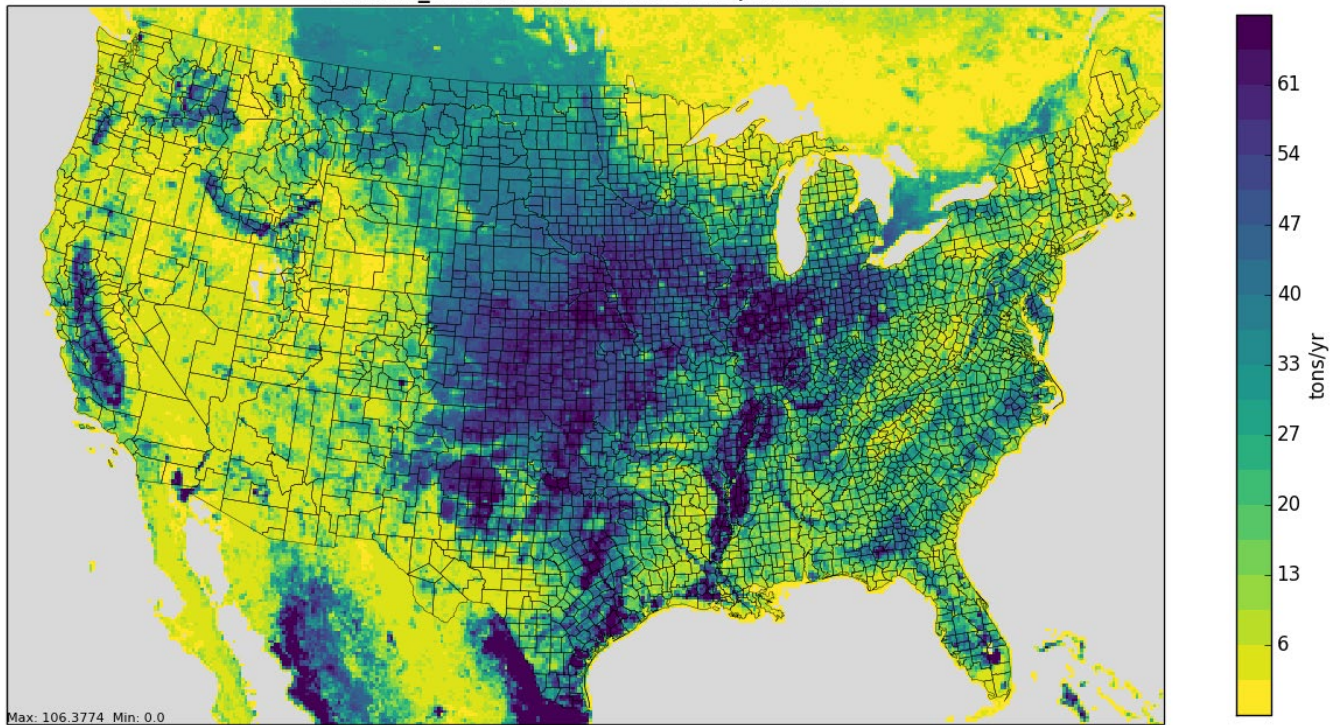


Figure 2-5. Annual isoprene emissions output from BEIS 3.61 for 2014

2014fa_nata beis ISOP emissions, annual

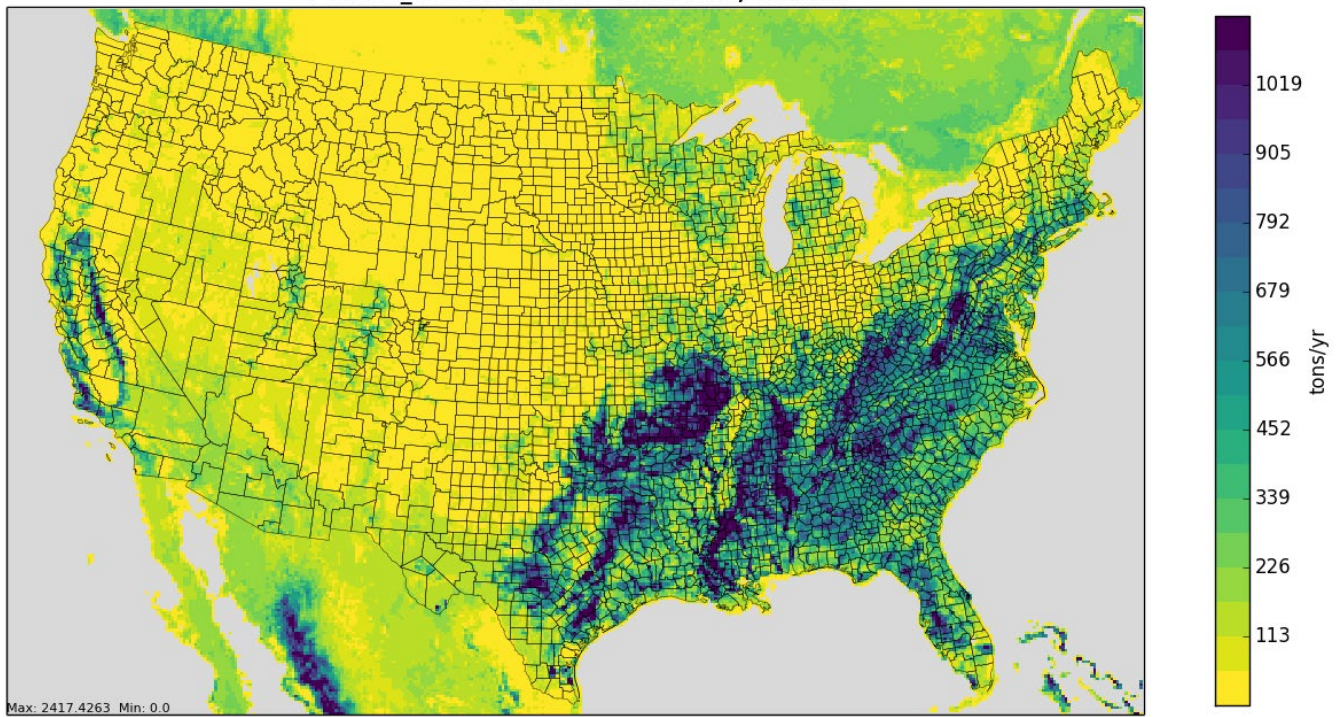


Figure 2-6. Annual acetaldehyde emissions output from BEIS 3.61 for 2014

2014fa_nata beis ALD2 emissions, annual

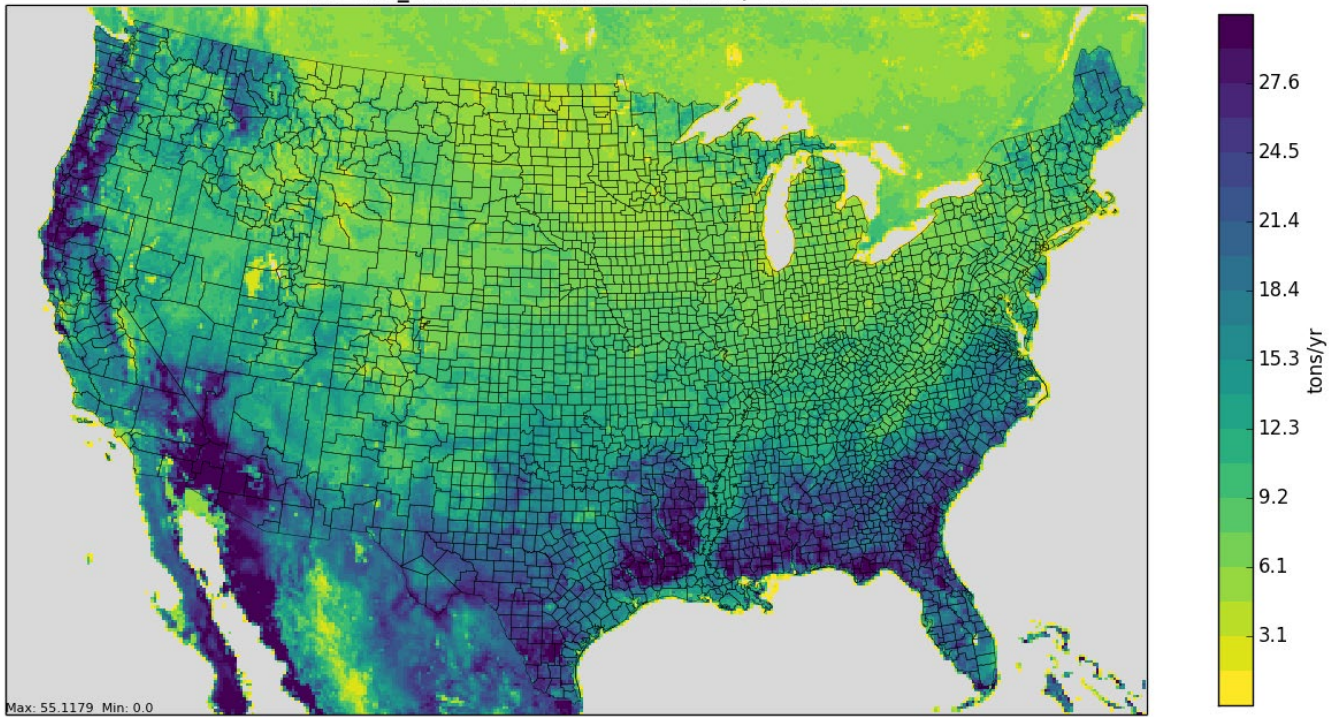
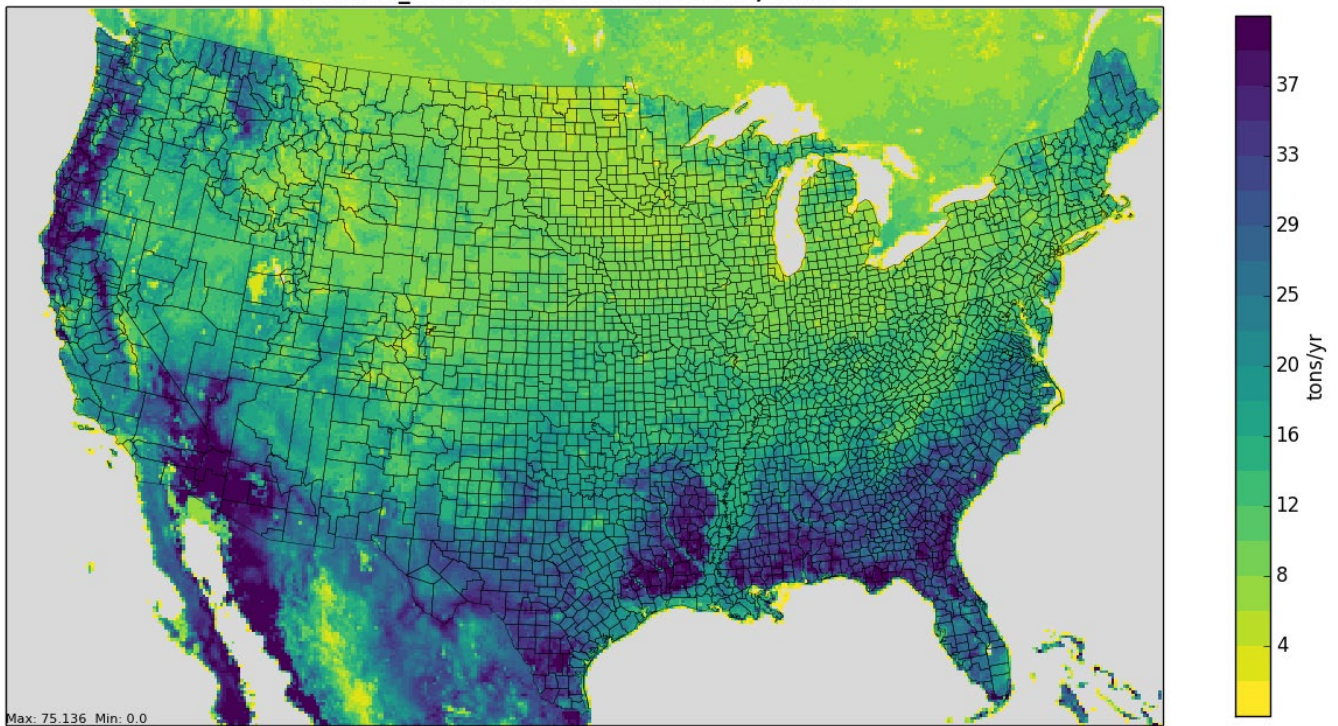


Figure 2-7. Annual formaldehyde emissions output from BEIS 3.61 for 2014

2014fa_nata beis FORM emissions, annual



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 2016 alpha platform are available from the Air Emissions Modeling website (<https://www.epa.gov/air-emissions-modeling/2016-alpha-platform>).

SMOKE version 4.5 was used to process the raw 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	
othafdust_adj	Surrogates	Yes	annual	
othar	Surrogates	Yes	annual & monthly	
onroad_can	Surrogates	Yes	monthly	
onroad_mex	Surrogates	Yes	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	

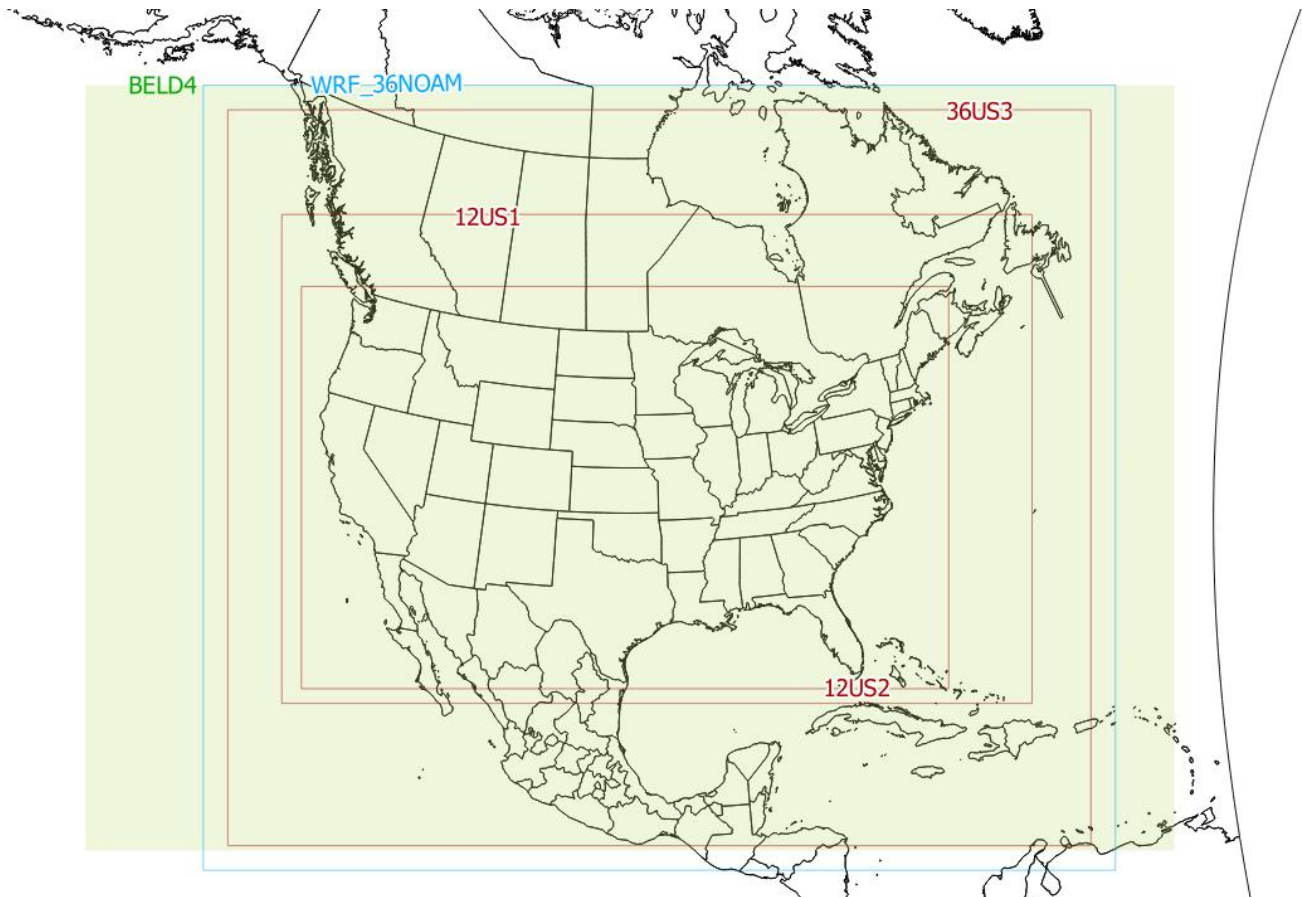
Biogenic emissions can be modeled two different ways in the CMAQ model. The BEIS model in SMOKE can produce gridded biogenic emissions that are then included in the gridded CMAQ-ready emissions inputs, or alternatively, CMAQ can be configured to create “in-line” biogenic emissions within CMAQ

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 three modeling domains: a 36-km resolution CONTINENTAL UNITED STATES “CONUS” modeling domain (36US3), and two 12-km resolution domains, 12US1 and 12US2. The domains are shown in Figure 3-1. Section 3.6 provides the details on the spatial surrogates and area-to-point data used to accomplish spatial allocation with SMOKE. More specifically, SMOKE was run on the 12US1 domain and emissions were extracted from 12US1 data files to create 12US2 emission.

Figure 3-1. Air quality modeling domains



All grids use a Lambert-Conformal projection, with Alpha = 33°, Beta = 45° and Gamma = -97°, with a center of X = -97° and Y = 40°. 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 36km grid	36 km	Entire conterminous US, almost all of Mexico, most of Canada (south of 60°N)	36US3	'LAM_40N97W', -2952000, -2772000, 36.D3, 36.D3, 172, 148, 1
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 2016 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. 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
	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

Inventory Pollutant	Model Species	Model species description
	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
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 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;

⁶ These emissions are created outside of SMOKE

- 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-specified 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 2016 alpha 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. Totals of each model species by state and sector can be found in the state-sector totals workbook for this 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 the 2016 platform because the ptfire and ptagfire inventories for 2016 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 integration⁷). 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 profiles⁸. SMOKE computes NONHAPTOG and then applies the speciation profiles to allocate the NONHAPTOG to the other air quality model VOC

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.

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). 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 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 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

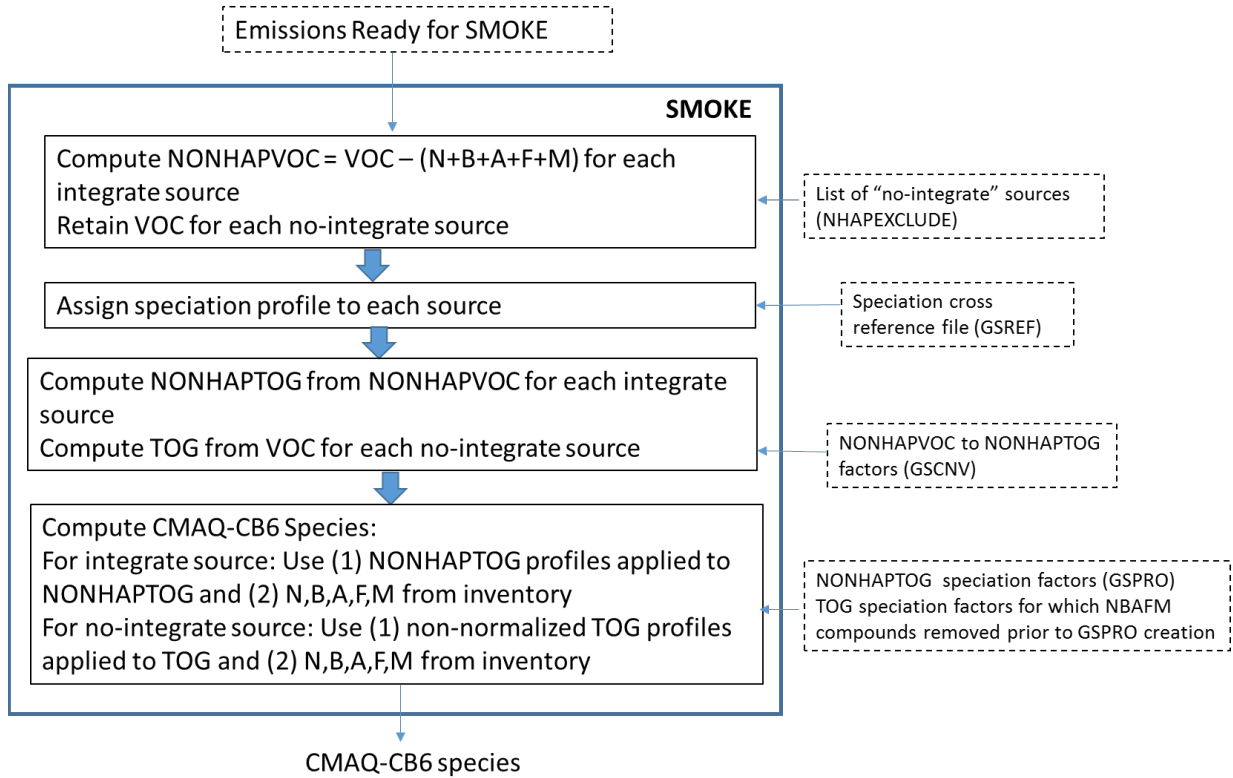


Table 3-4. Integration status of naphthalene, benzene, acetaldehyde, formaldehyde and methanol (NBAFM) for each platform sector

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)
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)

Platform Sector	Approach for Integrating NEI emissions of Naphthalene (N), Benzene (B), Acetaldehyde (A), Formaldehyde (F) and Methanol (M)
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 2016 alpha 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 the 2016 alpha platform 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 speciation¹⁰. Third, MOVES' internal speciation

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/>.

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) 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 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.

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) for these no-integrate sources.

For the biog sector, the speciation profiles used by BEIS are not included in SPECIATE. BEIS3.61 includes the species (SESQ), that is 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 2016 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)
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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	
PNC04_R	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 Gas 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 ptonipm 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 used for the 2016 Platform

Profile	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 D.

Table 3-8 summarizes the different profiles utilized for the fuel-related sources in each of the sectors for 2016. 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 2016

Sector	Sub-category	2014	
Nonroad- California & non US	gasoline exhaust	COMBO 8750a 8751a	Pre-Tier 2 E0 exhaust Pre-Tier 2 E10 exhaust
Nonroad-California	gasoline evaporative	COMBO 8753 8754	E0 evap E10 evap
Nonroad-California	gasoline refueling	COMBO 8869 8870	E0 Headspace 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 8870	E0 Headspace 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

Profile	Profile Description	Model Years	ProcessID	FuelSubTypeID	RegClassID
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

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

¹¹ 91 is the processed for APUs which are diesel engines not covered by the 2007 Heavy-Duty Rule, so the older technology applies 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.

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 speciation¹³. 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 with 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

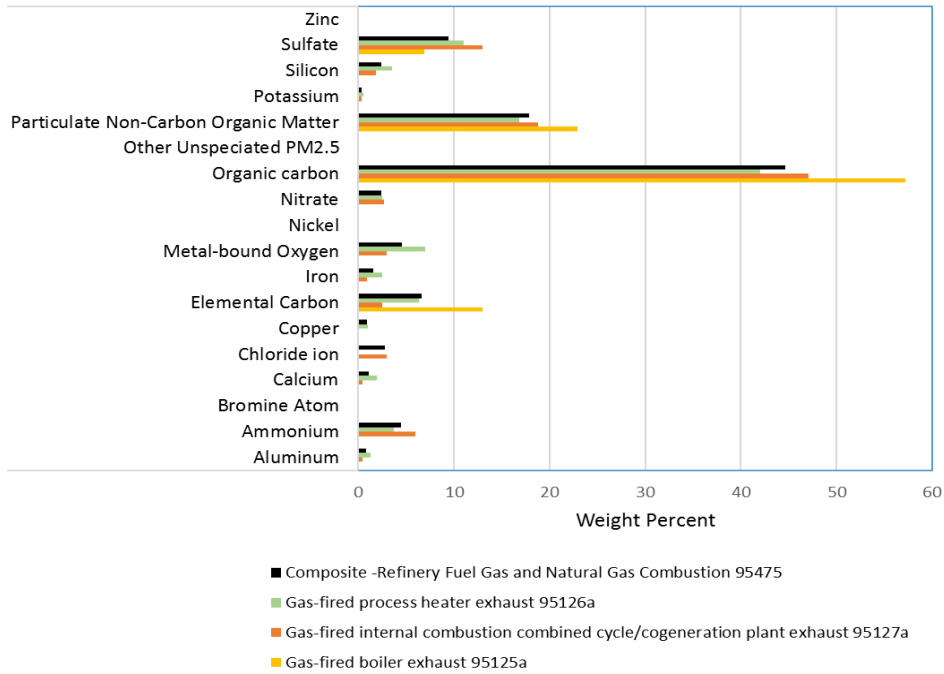
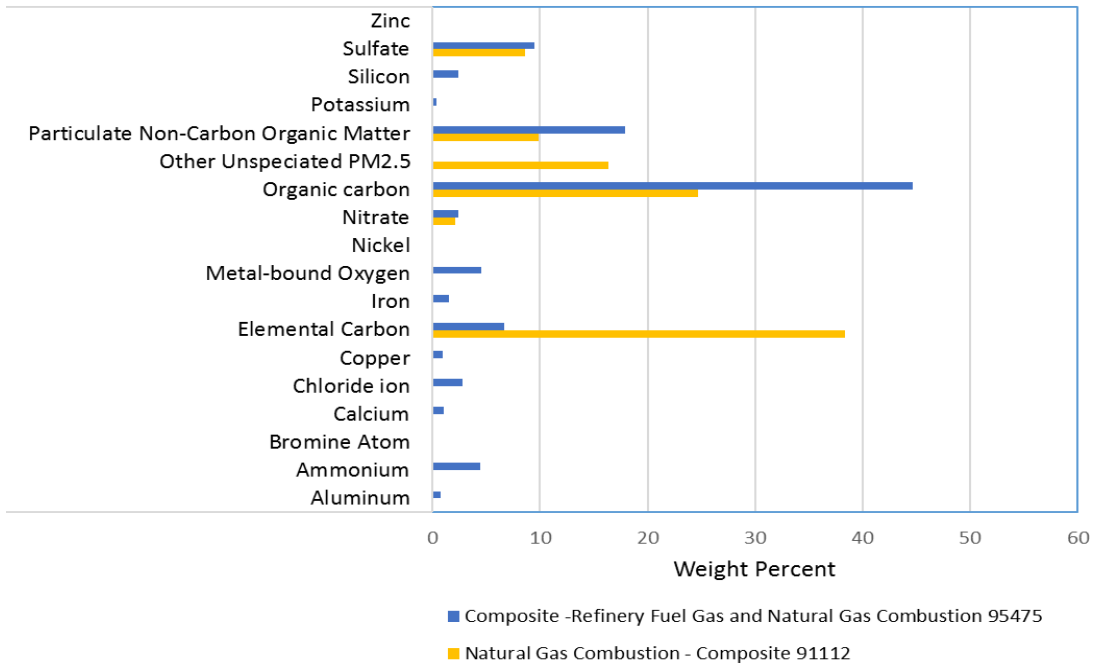


Figure 3-4. Comparison of PM profiles used for Natural gas combustion related sources



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., PM₁₀ 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 speciation¹⁴. 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:

$$\begin{aligned}
 \text{POC} &= 0.6395 * \text{PM25TIRE} + 0.0503 * \text{PM25BRAKE} \\
 \text{PEC} &= 0.0036 * \text{PM25TIRE} + 0.0128 * \text{PM25BRAKE}
 \end{aligned}$$

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/>.

$$\begin{aligned}
 \text{PNO3} &= 0.000 * \text{PM25TIRE} + 0.000 * \text{PM25BRAKE} \\
 \text{PSO4} &= 0.0 * \text{PM25TIRE} + 0.0 * \text{PM25BRAKE} \\
 \text{PNH4} &= 0.000 * \text{PM25TIRE} + 0.0000 * \text{PM25BRAKE} \\
 \text{PNCOM} &= 0.2558 * \text{PM25TIRE} + 0.0201 * \text{PM25BRAKE}
 \end{aligned}$$

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

NO_x emission factors and therefore NO_x inventories are developed on a NO₂ weight basis. For air quality modeling, NO_x is speciated into NO, NO₂, and/or HONO. For the non-mobile sources, the EPA used a single profile “NHONO” to split NO_x into NO and NO₂.

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 NO_x speciation for mobile sources. Based on tunnel studies, a HONO to NO_x 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, NO₂, 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 NO₂ fraction = 1 – NO – HONO. For more details on the NO_x fractions within MOVES, see <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
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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 SO₂ 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 SO₂ and relates the sulfate as a function of SO₂.

Sulfate is computed from SO₂ assuming that gaseous sulfate, which is comprised of many components, is primarily H₂SO₄. The equation for calculating H₂SO₄ is given below.

$$\begin{aligned} & \text{Emissions of SULF (as H}_2\text{SO}_4\text{)} \\ &= \text{SO}_2 \text{ emissions} \times \frac{\text{fraction of S emitted as sulfate}}{\text{fraction of S emitted as SO}_2} \times \frac{\text{MW H}_2\text{SO}_4}{\text{MW SO}_2} \end{aligned}$$

In the above, *MW* is the molecular weight of the compound. The molecular weights of H₂SO₄ and SO₂ are 98 g/mol and 64 g/mol, respectively.

This method does not reduce SO₂ 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 SO ₂	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. SO₂ 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	No	all	all	No
beis	Hourly	No	n/a	all	No
cmv_clc2	Annual	Yes	aveday	aveday	No
cmv_c3	Annual	Yes	aveday	aveday	No
nonpt	Annual	Yes	week	week	Yes
nonroad	Monthly	No	mwdss	mwdss	Yes
np_oilgas	Annual	Yes	week	week	Yes
onroad	Annual & monthly ¹	No	all	all	Yes

Platform sector short name	Inventory resolutions	Monthly profiles used?	Daily temporal approach	Merge processing approach	Process holidays as separate days
onroad_ca_adj	Annual & monthly ¹	No	all	all	Yes
othafdust_adj	Annual	Yes	week	all	No
othar	Annual & monthly	Yes	week	week	No
onroad_can	Monthly	No	week	week	No
onroad_mex	Monthly	No	week	week	No
othpt	Annual & monthly	Yes	mwdss	mwdss	No
pt_oilgas	Annual	Yes	mwdss	mwdss	Yes
ptegu	Annual & hourly	Yes ²	all	all	No
ptnonipm	Annual	Yes	mwdss	mwdss	Yes
ptagfire	Daily	No	all	all	No
ptfire	Daily	No	all	all	No
ptfire_othna	Daily	No	all	all	No
rail	Annual	Yes	aveday	aveday	No
rwc	Annual	No ³	met-based ³	all	No ³

¹Note 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.

²Only units that do not have matching hourly CEMS data use monthly temporal profiles.

³Except for 2 SCCs that do not use met-based speciation

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 2016 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 2016 because the CEMS data replaces the NO_x and SO₂ 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

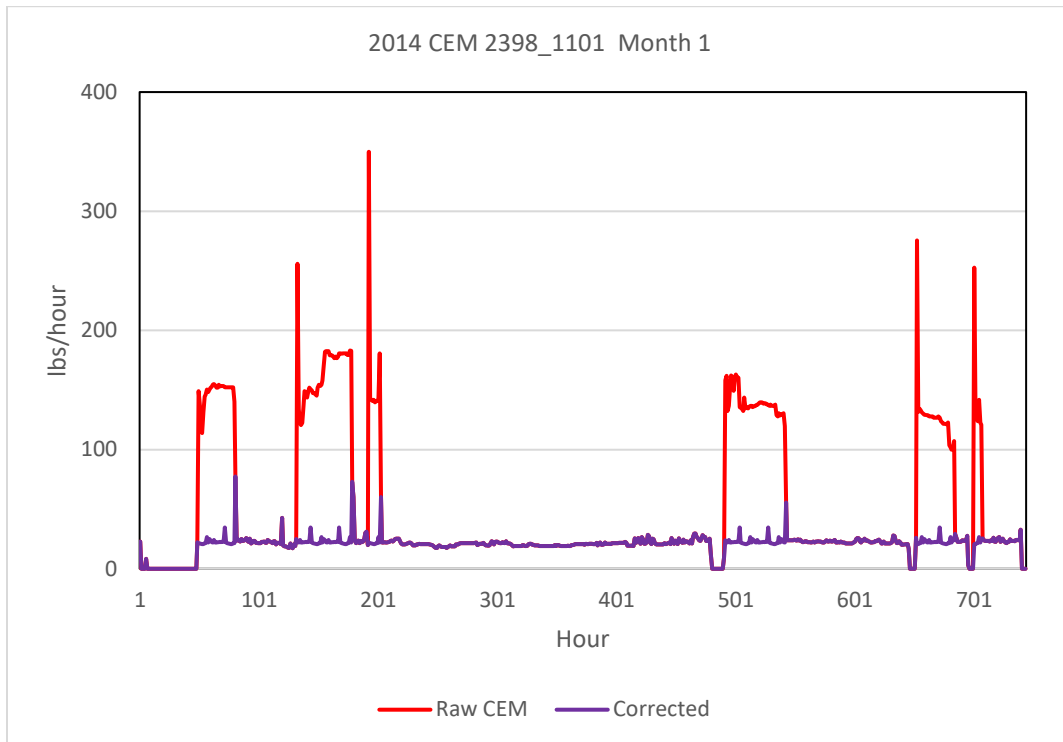
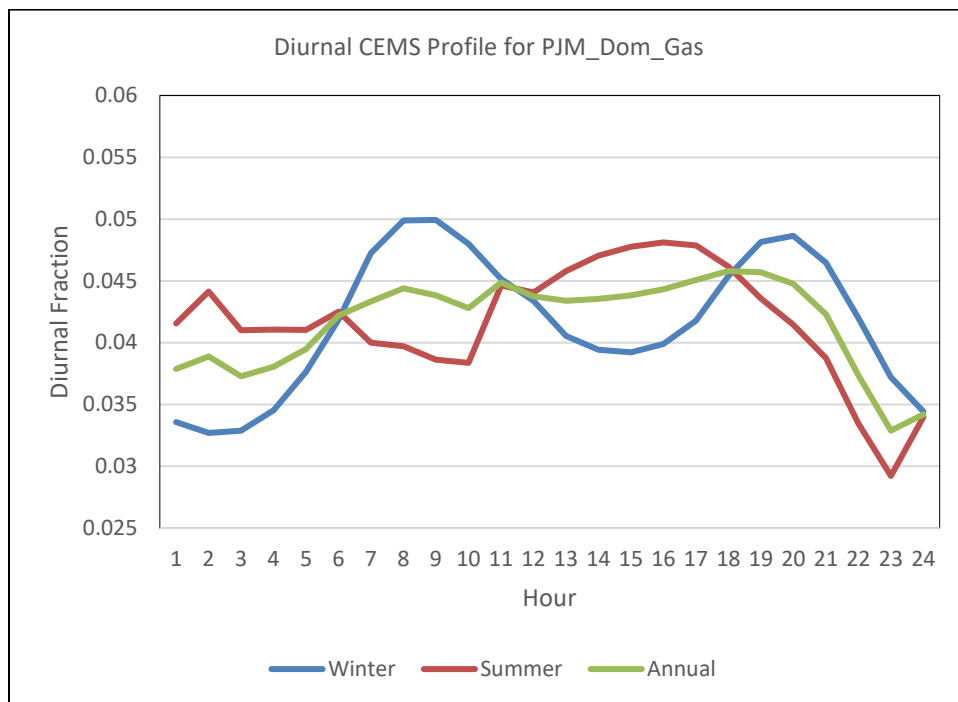


Figure 3-6. Seasonal diurnal profiles for EGU emissions in a Virginia Region



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 2016 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, SO₂, 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 SO₂ CEMS data are used to allocate NO_x and SO₂ 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 2016 CEMS heat 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 SO₂ CEMS data are used to replace inventory NO_x and SO₂ 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 SO₂, 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 SO₂) 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., 2016 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

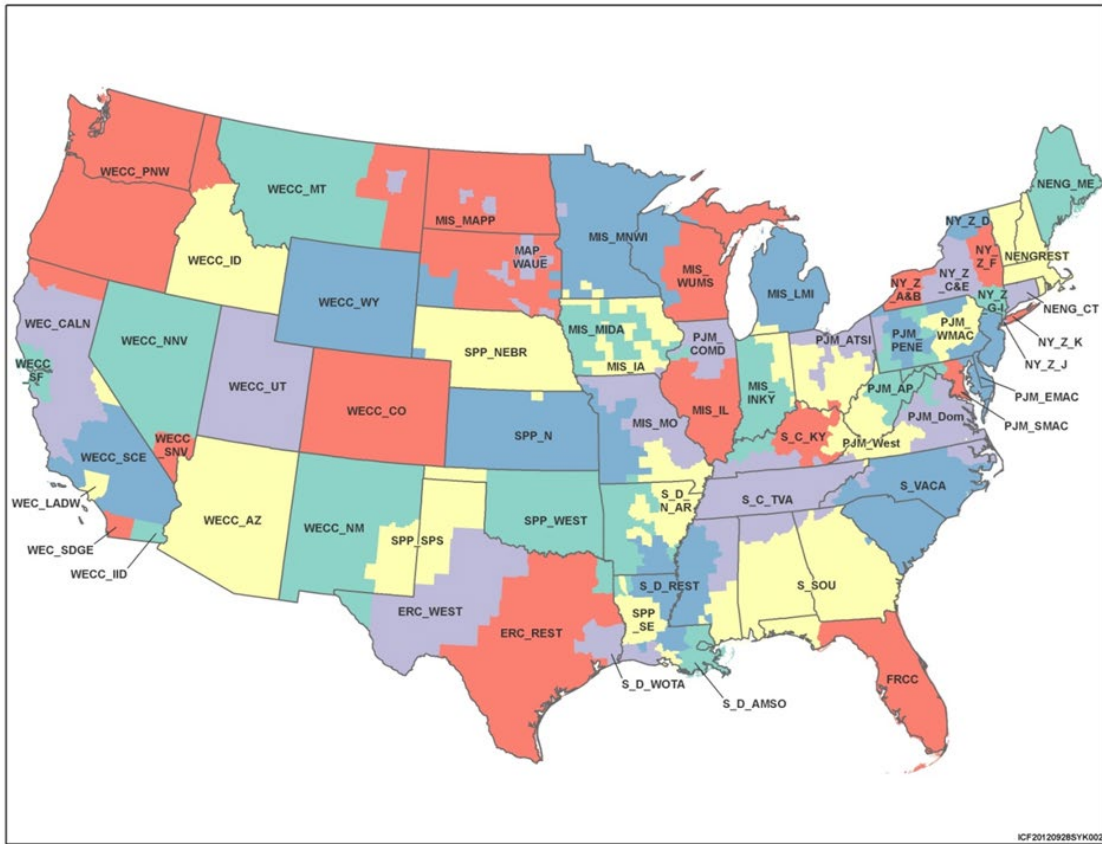
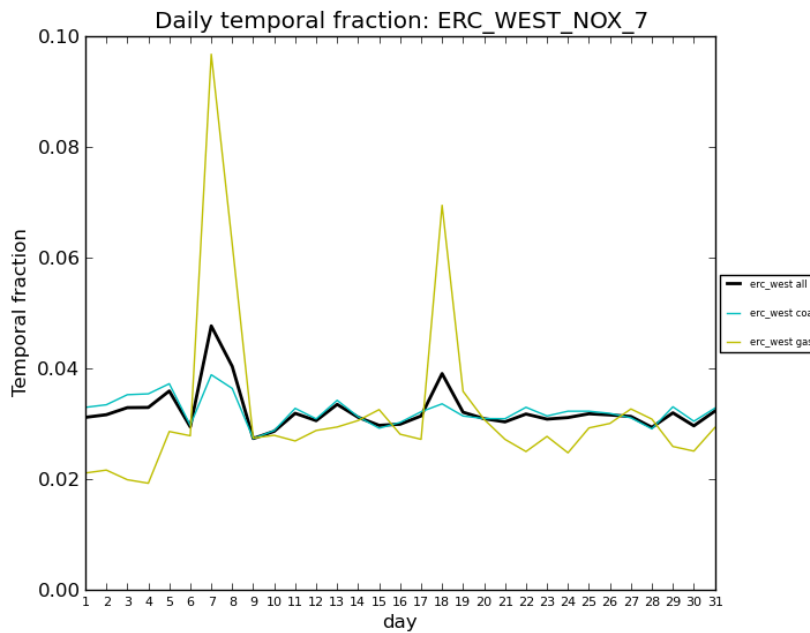


Figure 3-8. Month-to-day profiles for different fuels in a West Texas Region



3.3.3 Airport Temporal allocation (ptnonipm)

Airport temporal profiles were updated in 2014v7.0 and were kept the same for 2014v7.1 and 2016 alpha 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

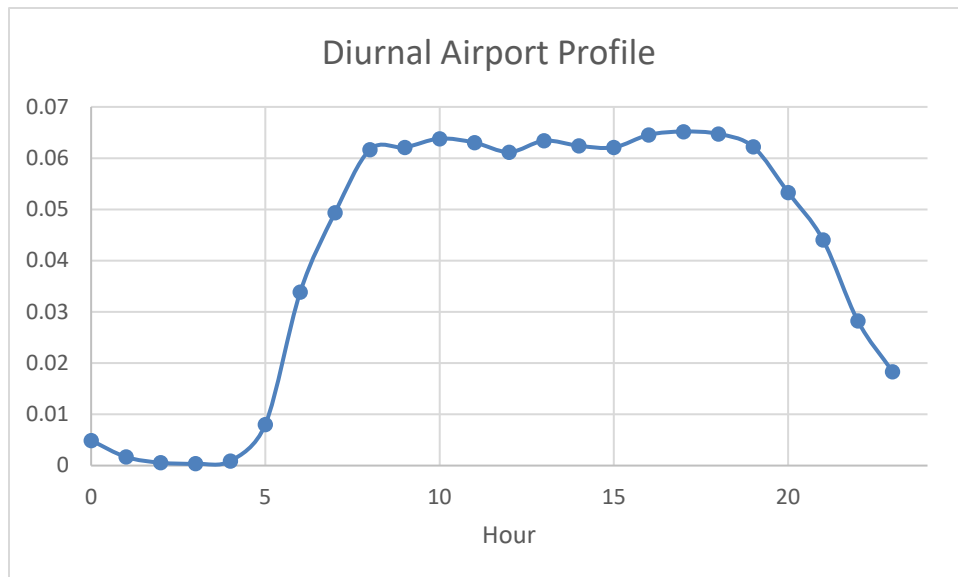


Figure 3-10. Weekly profile for all Airport SCCs

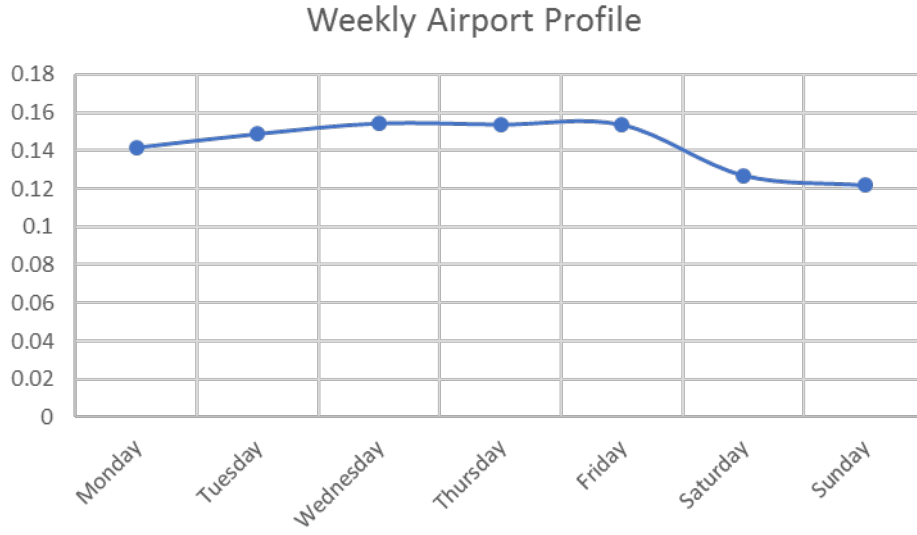


Figure 3-11. Monthly Profile for all Airport SCCs

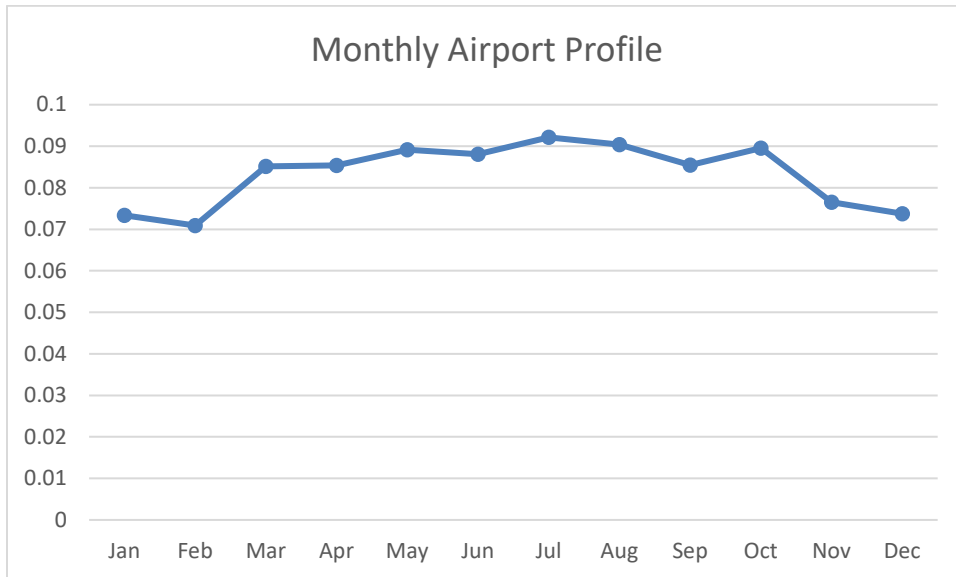
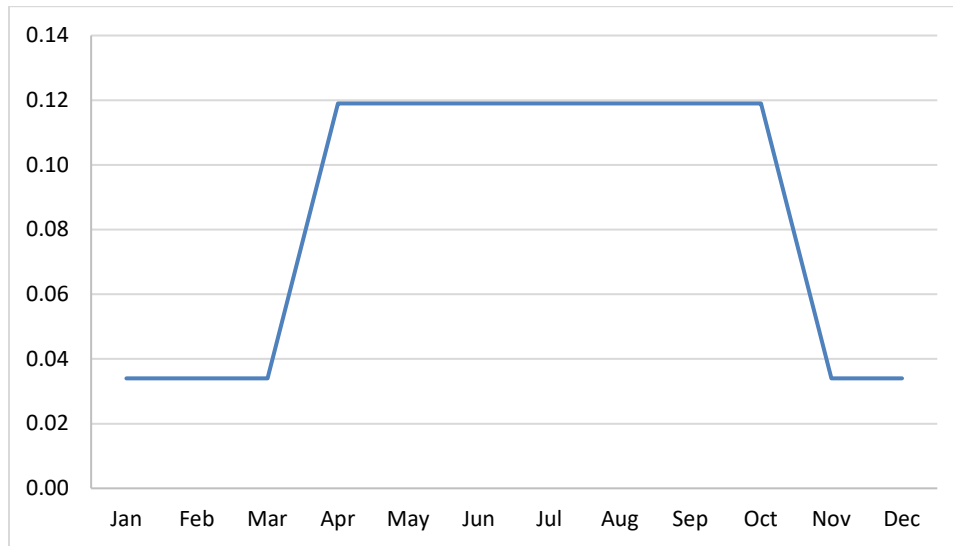


Figure 3-12. Alaska Seaplane Profile



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 NH₃; 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.

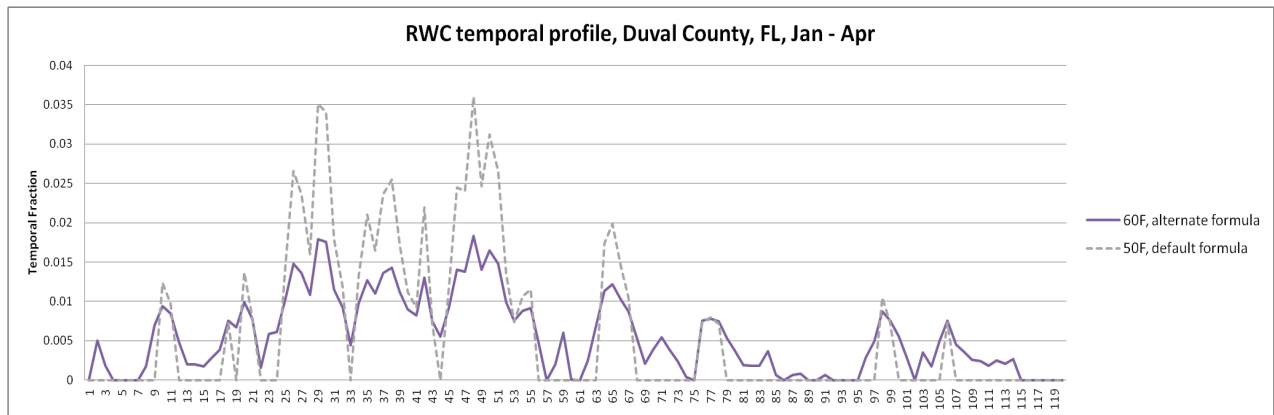
Gentpro reads in gridded meteorological data (output from MCIP) along with spatial surrogates and uses the specified algorithm to produce a new temporal profile that can be input into SMOKE. The meteorological variables and the resolution of the generated temporal profile (hourly, daily, etc.) depend 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.

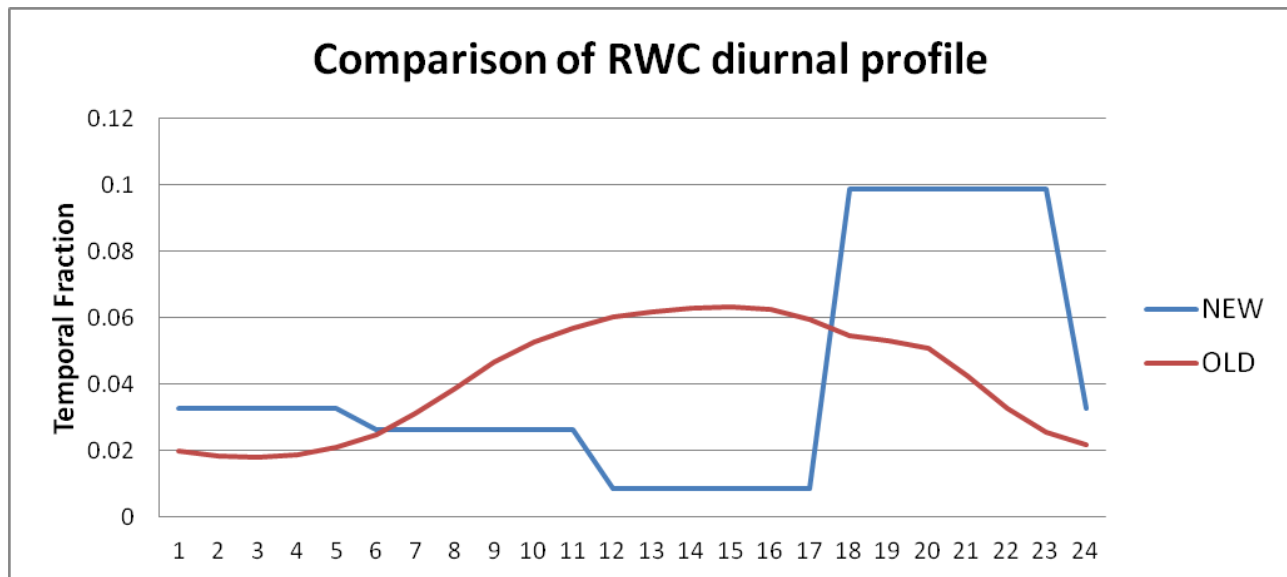
Figure 3-13 illustrates the impact of changing the temperature threshold for a warm climate county. The plot shows the temporal fraction by day for Duval County, Florida, for the first four months of 2007. The default 50 °F threshold creates large spikes on a few days, while the 60 °F threshold dampens 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 (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.

Data used to produce the diurnal profile for OHH, shown in Figure 3-15, are 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. Data used to produce the diurnal profile for OHH, based on heat load (BTU/hr)

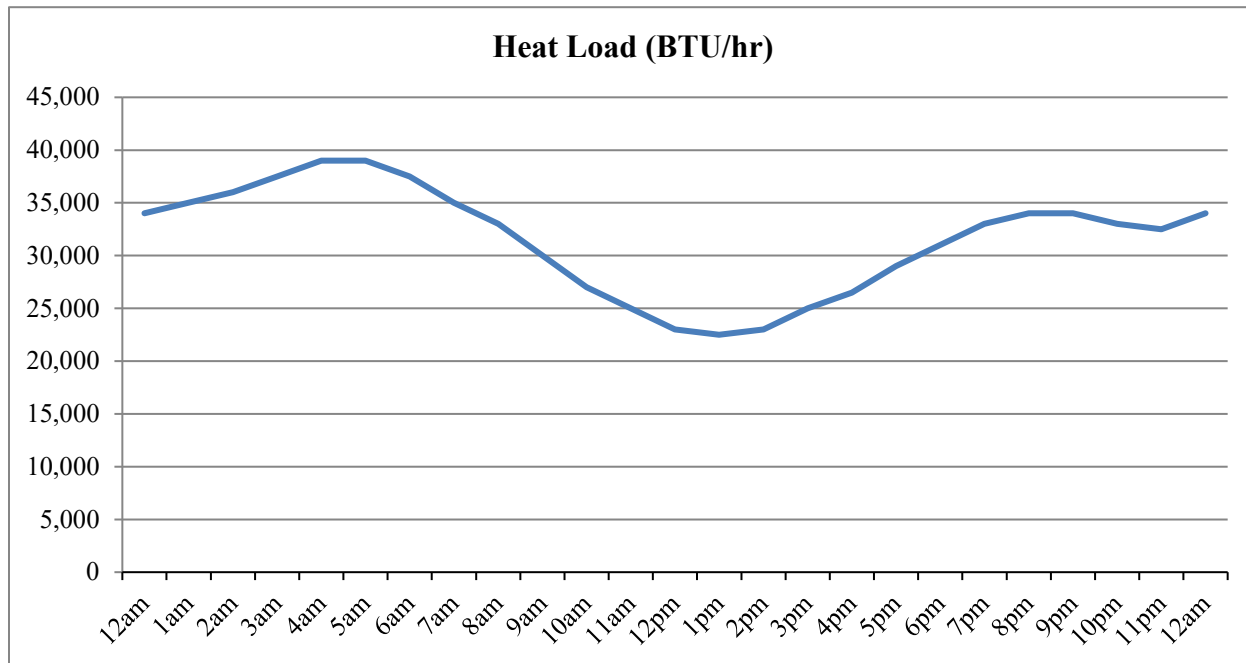


Figure 3-16. Day-of-week temporal profiles for OHH and Recreational RWC

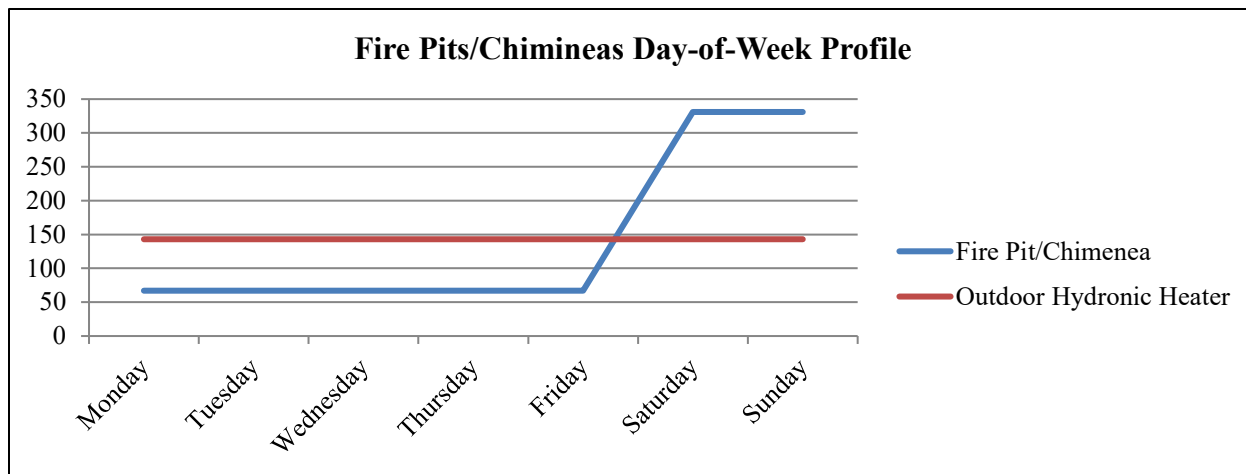
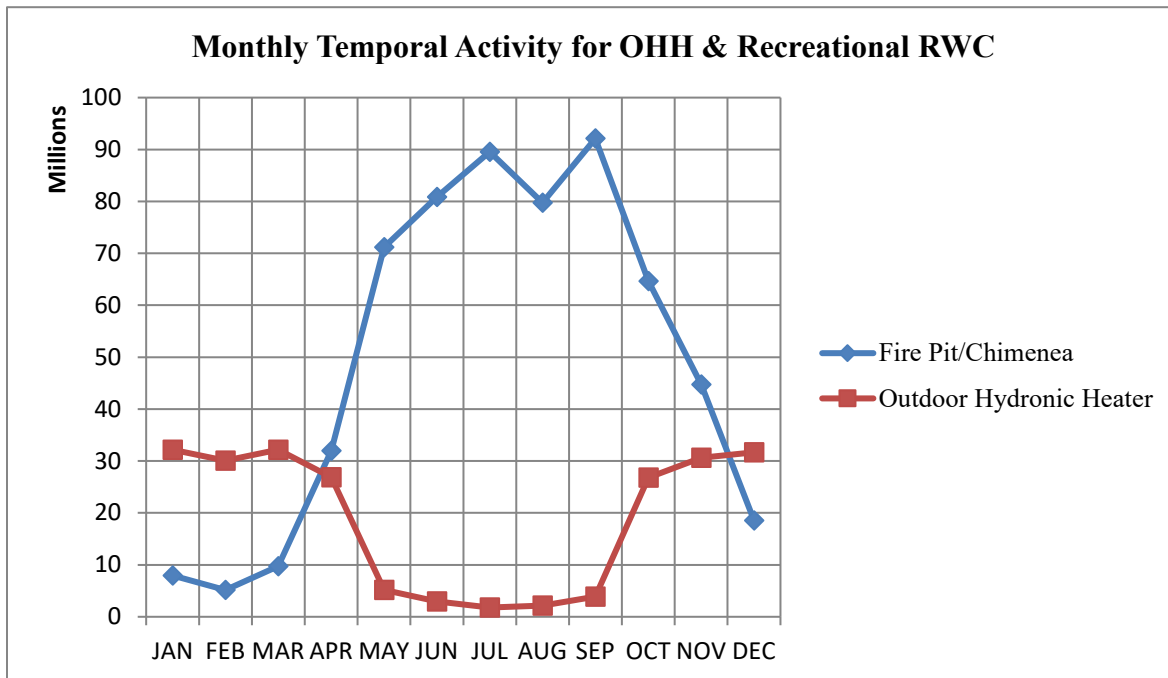


Figure 3-17. Annual-to-month temporal profiles for OHH and recreational RWC



3.3.5 Agricultural Ammonia Temporal Profiles (ag)

For the agricultural livestock NH₃ 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 NH₃ emission variations from livestock as a function of ambient temperature, aerodynamic resistance, and wind speed. The equations are:

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

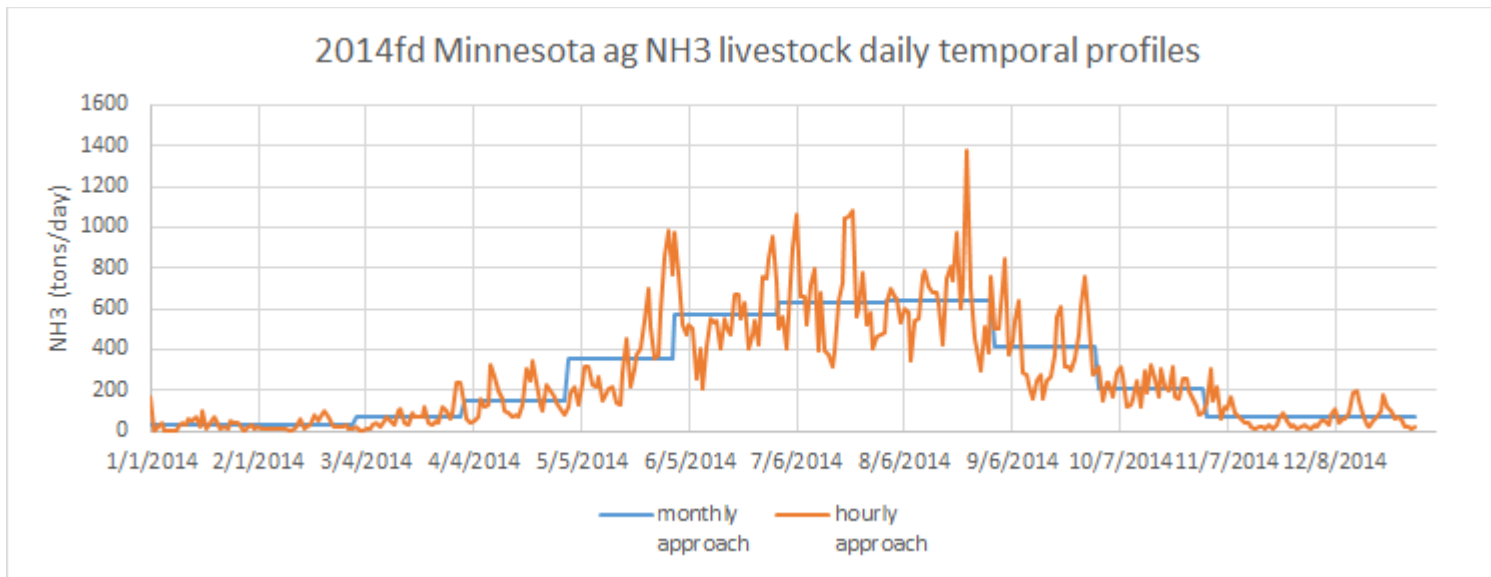
$$PE_{i,h} = E_{i,h} / \text{Sum}(E_{i,h})$$

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 NH₃ emissions temporal allocation approach, summed to daily emissions



For the 2016 alpha platform, the GenTPRO approach is applied to all sources in the ag sector, NH₃ and non- NH₃, 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 2016. Therefore, in the 2016 alpha 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.

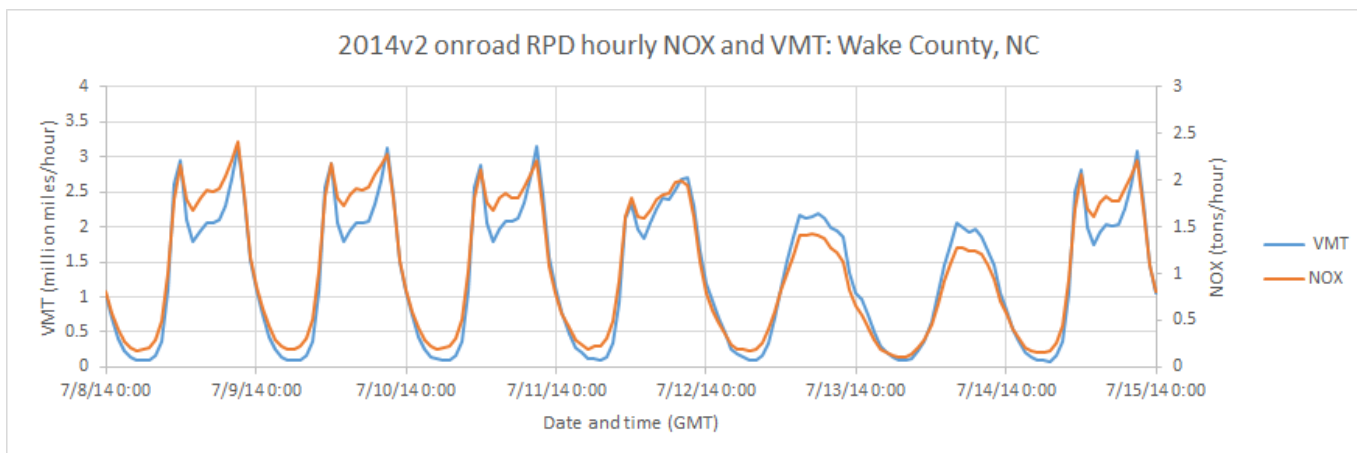
The “inventories” referred to in Table 3-18 consist of activity data for the onroad sector, not emissions. For the off-network emissions from the RPP and RPV processes, the VPOP activity data is annual and does not need temporal allocation. For processes that result from hoteling of combination trucks (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

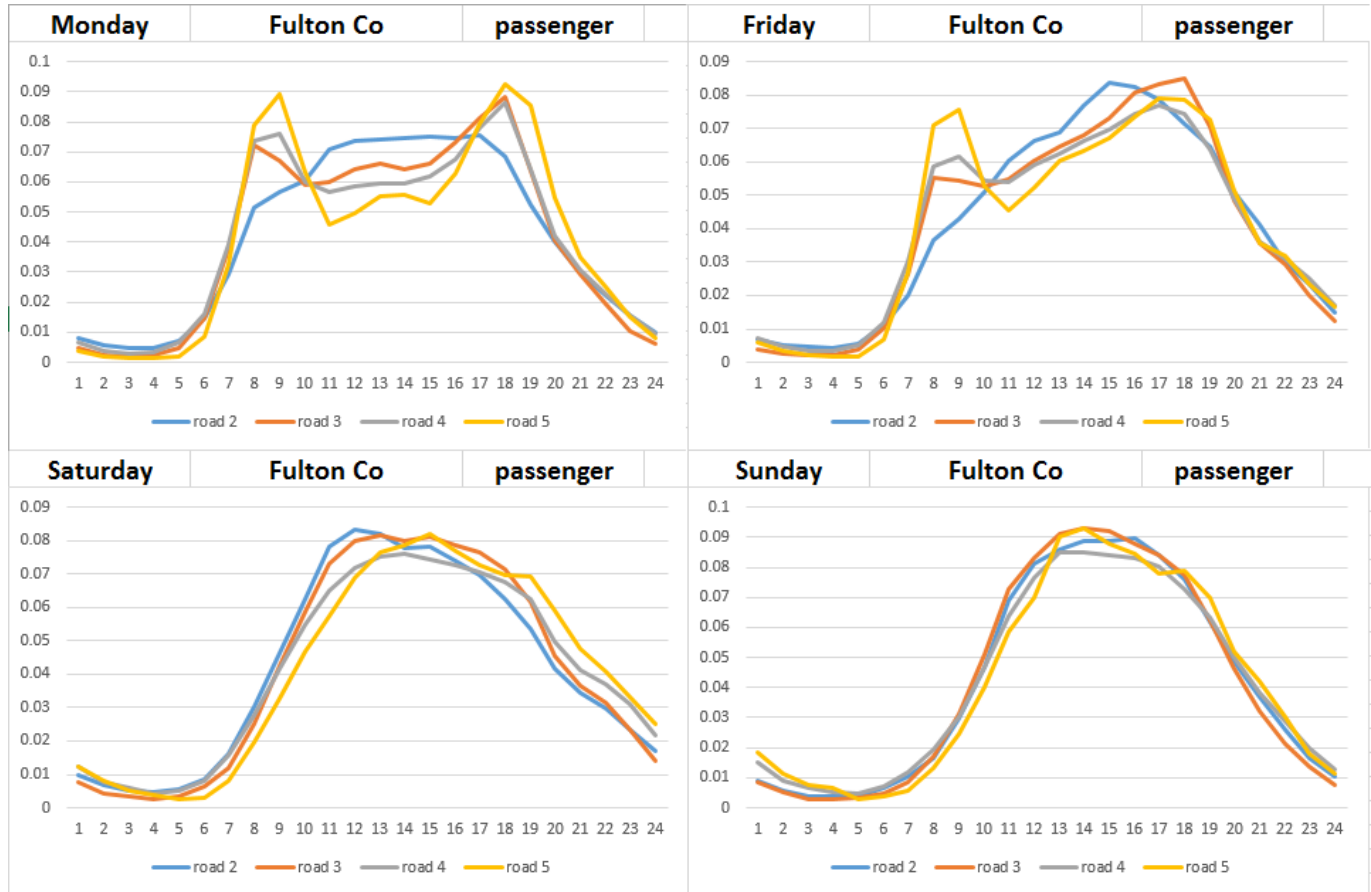
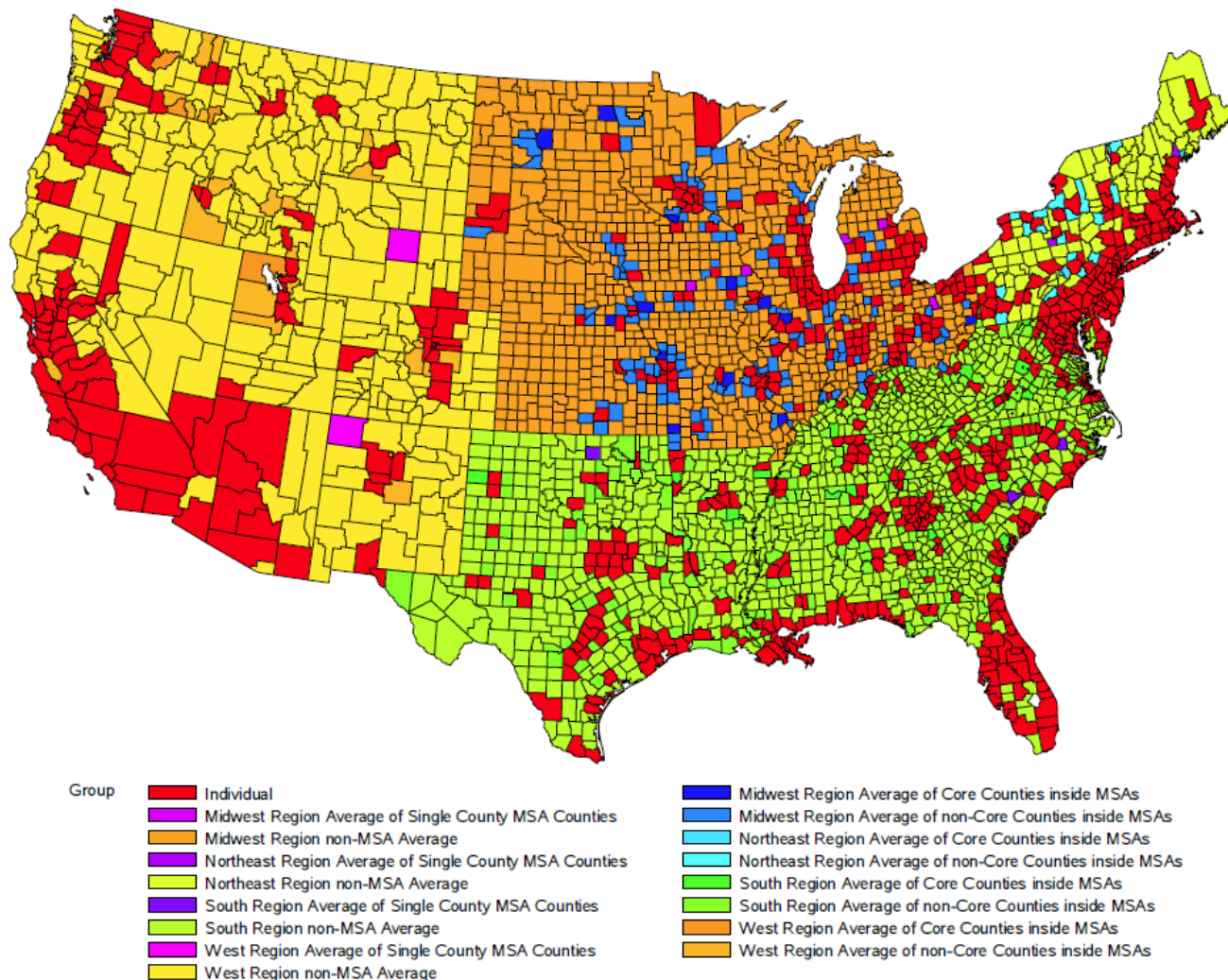


Figure 3-21. Counties for which MOVES Speeds and Temporal Profiles could be Populated

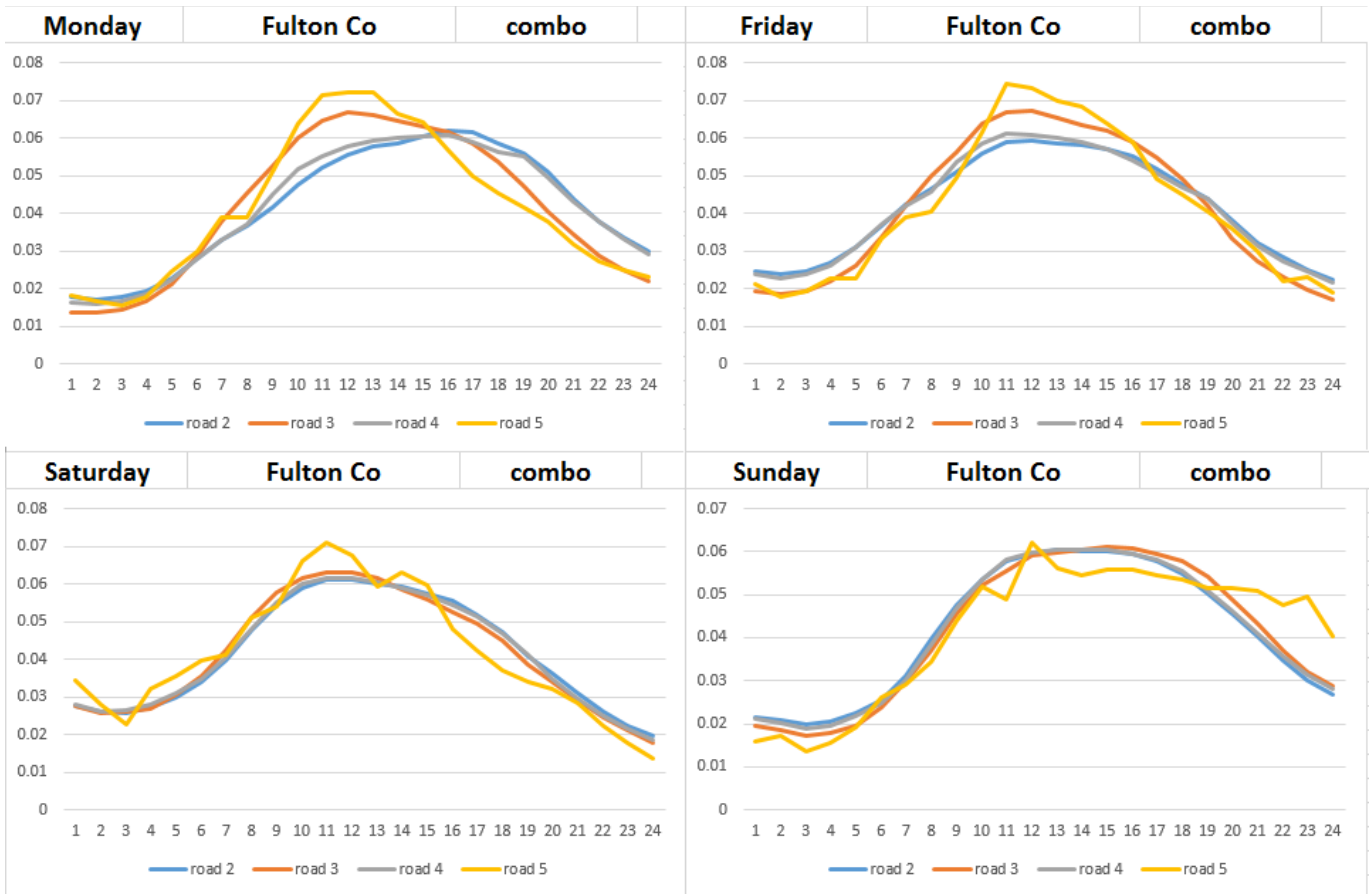


For hoteling, day-of-week profiles are the same as non-hoteling for combination trucks, while hour-of-day non-hoteling profiles for combination trucks were inverted to create new hoteling profiles that peak overnight instead of during the day. The combination truck profiles for Fulton County are shown 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 week¹⁵, 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 for 2016, 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 from different grid resolutions. For this reason, to ensure consistency between grid resolutions, afdust emissions for the 36US3 grid are aggregated from the 12US1 emissions. Application of the transport fraction and meteorological adjustments prevents the overestimation of fugitive dust impacts in the grid modeling as compared to ambient samples.

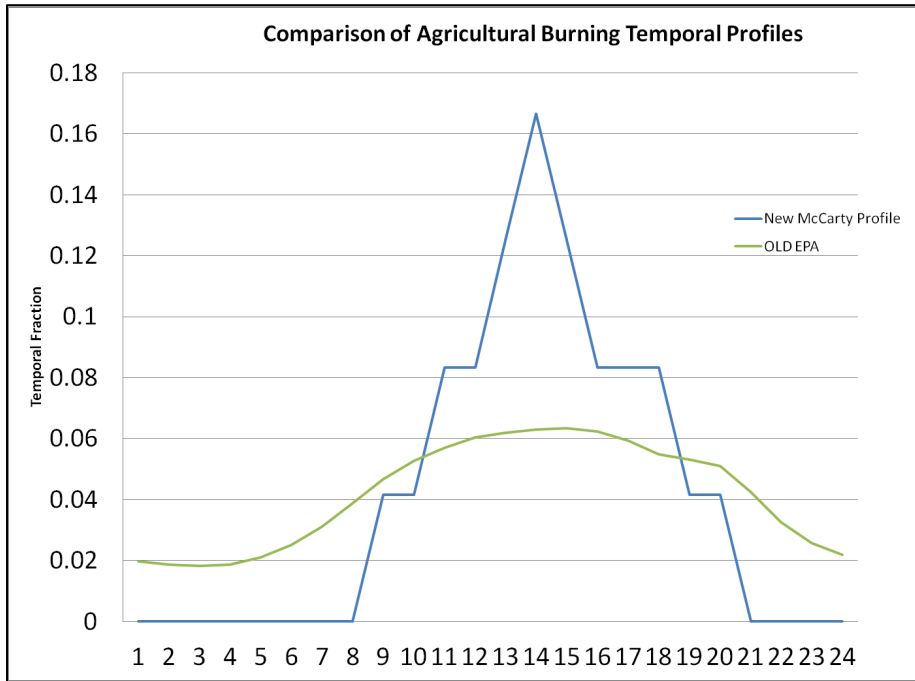
Biogenic emissions in the beis sector vary by every day of the year because they are developed using meteorological data including temperature, surface pressure, and radiation/cloud data. The emissions are computed using appropriate emission factors according to the vegetation in each model grid cell, 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 NO_x 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 NO_x 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 2016 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.

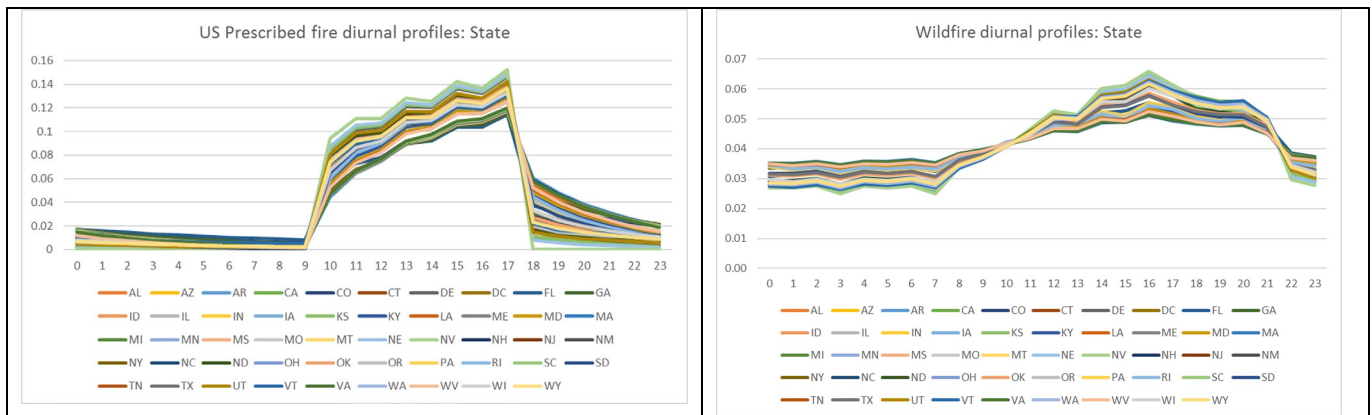
Figure 3-23. Agricultural burning diurnal temporal profile



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 2016 alpha platform uses the ptfire diurnal profiles from 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 a national 36-km domain and two national 12-km domains. To accomplish this, SMOKE used national 36-km and 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 36-km and 12-km surrogates cover the entire CONUS domain 12US1 shown in Figure 3-1. The 36US3 domain includes a portion of Alaska, and since Alaska emissions are typically not included in air quality modeling, special considerations are taken to include Alaska emissions in 36-km modeling.

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 an 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 2016 alpha 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 2016 alpha 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 2016 alpha 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	<i>Housing</i>	507	<i>Heavy Light Construction Industrial Land</i>
131	<i>urban Housing</i>	510	<i>Commercial plus Industrial</i>
132	<i>Suburban Housing</i>	515	<i>Commercial plus Institutional Land</i>
134	<i>Rural Housing</i>	520	<i>Commercial plus Industrial plus Institutional</i>
137	<i>Housing Change</i>		<i>Golf Courses plus Institutional plus</i>
140	<i>Housing Change and Population</i>	525	<i>Industrial plus Commercial</i>
150	Residential Heating – Natural Gas	526	<i>Residential – Non-Institutional</i>
160	<i>Residential Heating – Wood</i>	527	<i>Single Family Residential</i>
170	Residential Heating – Distillate Oil		Residential + Commercial + Industrial +
180	Residential Heating – Coal	535	Institutional + Government
190	Residential Heating – LP Gas	540	<i>Retail Trade (COM1)</i>
201	<i>Urban Restricted Road Miles</i>	545	<i>Personal Repair (COM3)</i>
202	Urban Restricted AADT		<i>Professional/Technical (COM4) plus General</i>
205	Extended Idle Locations	555	<i>Government (GOV1)</i>
211	<i>Rural Restricted Road Miles</i>	560	Hospital (COM6)
212	<i>Rural Restricted AADT</i>		<i>Light and High Tech Industrial (IND2 +</i>
221	<i>Urban Unrestricted Road Miles</i>	575	<i>IND5)</i>
222	<i>Urban Unrestricted AADT</i>	580	<i>Food Drug Chemical Industrial (IND3)</i>
231	<i>Rural Unrestricted Road Miles</i>	585	<i>Metals and Minerals Industrial (IND4)</i>
232	<i>Rural Unrestricted AADT</i>	590	<i>Heavy Industrial (IND1)</i>
239	Total Road AADT	595	<i>Light Industrial (IND2)</i>
240	Total Road Miles	596	<i>Industrial plus Institutional plus Hospitals</i>
241	<i>Total Restricted Road Miles</i>	650	Refineries and Tank Farms
242	All Restricted AADT	670	Spud Count – CBM Wells
243	<i>Total Unrestricted Road Miles</i>	671	Spud Count – Gas Wells
244	All Unrestricted AADT	672	Gas Production at Oil Wells
258	Intercity Bus Terminals	673	Oil Production at CBM Wells
259	Transit Bus Terminals	674	Unconventional Well Completion Counts
260	<i>Total Railroad Miles</i>	676	<i>Well Count – All Producing</i>
261	NTAD Total Railroad Density	677	<i>Well Count – All Exploratory</i>
271	NTAD Class 1 2 3 Railroad Density	678	Completions at Gas Wells
272	<i>NTAD Amtrak Railroad Density</i>	679	Completions at CBM Wells
		681	Spud Count – Oil Wells
		683	Produced Water at All Wells
		685	Completions at Oil Wells
		686	<i>Completions at All Wells</i>

Code	Surrogate Description	Code	Surrogate Description
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
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 2016 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 2014. 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 2016 alpha 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., NH₃, NO_x, PM_{2.5}, SO₂, and VOC) by sector assigned to each spatial surrogate.

Table 3-22. Selected 2016 CAP emissions by sector for U.S. Surrogates (CONUS 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	2,776,255	--	--	--	179,970
cmv_c1c2	808	2013 Shipping Density	293	520,571	14,357	421	9,117
cmv_c1c2	820	Ports NEI2014 Activity	11	23,201	729	148	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	2,380	246	2	457
nonroad	304	NLCD Open + Low	4	2,028	177	5	2,914
nonroad	305	NLCD Low + Med	114	19,450	4,654	154	136,612

Sector	ID	Description	NH3	NOX	PM2_5	SO2	VOC
nonroad	306	NLCD Med + High	346	207,923	13,328	431	113,689
nonroad	307	NLCD All Development	104	34,233	15,676	124	169,016
nonroad	308	NLCD Low + Med + High	684	378,335	31,078	506	63,783
nonroad	309	NLCD Open + Low + Med	113	20,838	1,250	152	42,930
nonroad	310	NLCD Total Agriculture	493	369,213	26,906	390	43,497
nonroad	320	NLCD Forest Land	19	6,306	1,153	16	8,386
nonroad	321	NLCD Recreational Land	161	22,718	13,568	235	500,251
nonroad	350	NLCD Water	216	142,165	7,301	391	380,972
nonroad	850	Golf Courses	13	2,027	117	18	5,603
nonroad	860	Mines	2	2,670	271	2	516
np_oilgas	670	Spud Count - CBM Wells	0	0	0	0	155
np_oilgas	671	Spud Count - Gas Wells	0	0	0	0	9,775
np_oilgas	672	Gas Production at Oil Wells	0	2,890	0	21,703	117,295
np_oilgas	673	Oil Production at CBM Wells	0	52	0	0	3,033
np_oilgas	674	Unconventional Well Completion Counts	0	47,074	1,793	237	3,402
np_oilgas	678	Completions at Gas Wells	0	3,384	26	6,768	71,343
np_oilgas	679	Completions at CBM Wells	0	11	0	483	1,366
np_oilgas	681	Spud Count - Oil Wells	0	0	0	0	65,351
np_oilgas	683	Produced Water at All Wells	0	11	0	0	87,045
np_oilgas	685	Completions at Oil Wells	0	3,000	129	2,266	50,750
np_oilgas	687	Feet Drilled at All Wells	0	114,998	3,995	449	9,059
np_oilgas	691	Well Counts - CBM Wells	0	28,093	483	12	23,454
np_oilgas	692	Spud Count - All Wells	0	9,018	255	113	365
np_oilgas	693	Well Count - All Wells	0	0	0	0	186
np_oilgas	694	Oil Production at Oil Wells	0	4,874	0	6,337	1,049,085
np_oilgas	695	Well Count - Oil Wells	0	110,111	2,892	80	408,969
np_oilgas	696	Gas Production at Gas Wells	0	45,335	2,123	163	57,017
np_oilgas	697	Oil Production at Gas Wells	0	1,346	0	25	359,070
np_oilgas	698	Well Count - Gas Wells	15	303,844	5,457	299	665,379
np_oilgas	699	Gas Production at CBM Wells	0	2,151	325	26	4,179
onroad	205	Extended Idle Locations	521	184,705	2,170	74	34,050
onroad	239	Total Road AADT	0	0	0	0	5,935
onroad	242	All Restricted AADT	35,739	1,285,235	40,512	8,435	200,706
onroad	244	All Unrestricted AADT	64,970	1,929,919	75,206	17,813	514,332
onroad	258	Intercity Bus Terminals	0	142	2	0	33
onroad	259	Transit Bus Terminals	0	88	4	0	192
onroad	304	NLCD Open + Low	0	773	17	1	2,546
onroad	306	NLCD Med + High	0	15,208	278	18	17,358
onroad	307	NLCD All Development	0	589,660	11,395	953	1,128,888
onroad	308	NLCD Low + Med + High	0	39,617	662	61	57,232
onroad	506	Education	0	489	17	1	721
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

Sector	ID	Description	NH3	NOX	PM2_5	SO2	VOC
rwc	300	NLCD Low Intensity Development	15,331	30,493	313,945	7,684	338,465

For 36US3 modeling, most U.S. emissions sectors were processed using 36-km spatial surrogates, and if applicable, 36-km meteorology. Exceptions include:

- For the onroad and onroad_ca_adj sectors, 36US3 emissions were aggregated from 12US1 by summing emissions from a 3x3 group of 12-km cells into a single 36-km cell. Differences in 12-km and 36-km meteorology can introduce differences in onroad emissions, and so this approach ensures that the 36-km and 12-km onroad emissions are consistent. However, this approach means that 36US3 onroad does not include emissions in Southeast Alaska; therefore, Alaska onroad emissions are included in the Canadian onroad sector (onroad_can), as described in Section 2.5.3. The 36US3 onroad_can emissions, including Canada and Alaska, are spatially allocated using 36-km surrogates and processed with 36-km meteorology.
- Similarly to onroad, because afdust emissions incorporate meteorologically-based adjustments, afdust_adj emissions for 36US3 were aggregated from 12US1 to ensure consistency in emissions between modeling domains. Again, similarly to onroad, this means 36US3 afdust does not include emissions in Southeast Alaska; therefore, Alaska afdust emissions are included in the Canadian dust sector (othafdust_adj), as described in Section 2.5.2. The 36US3 othafdust_adj emissions, including Canada and Alaska, are spatially allocated using 36-km surrogates and adjusted with 36-km meteorology.
- The ag and rwc sectors are processed using 36-km spatial surrogates, but using temporal profiles based on 12-km meteorology.

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 have been updated in the 2014v7.1 platform and carried forward into the 2016 alpha 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 Municipal 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

Code	Mexican or Canadian Surrogate Description	NH ₃	NO _x	PM _{2.5}	SO ₂	VOC
11	MEX 2015 Population	26,410	125,626	4,309	495	143,747
14	MEX Residential Heating - Wood	0	1,335	17,124	204	117,737
16	MEX Residential Heating - Distillate Oil	0	13	0	3	0
20	MEX Residential Heating - LP Gas	0	5,500	165	0	93
22	MEX Total Road Miles	2,789	361,522	10,292	6,079	72,731
24	MEX Total Railroads Miles	0	24,326	543	213	948
26	MEX Total Agriculture	175,112	134,919	28,631	6,455	10,855
32	MEX Commercial Land	0	75	1,653	0	25,416
34	MEX Industrial Land	4	1,138	2,005	0	121,933
36	MEX Commercial plus Industrial Land	0	2,218	30	6	100,789
38	MEX Commercial plus Institutional Land	2	1,645	70	3	45
40	MEX Residential (RES1-4)+Comercial+Industrial+Institutional+Government	0	4	11	0	77,571
42	MEX Personal Repair (COM3)	0	0	0	0	5,841
44	MEX Airports Area	0	3,708	105	480	1,270
50	MEX Mobile sources - Border Crossing	5	161	1	3	293
100	CAN Population	740	66	764	14	343
101	CAN total dwelling	408	35,196	2,578	4,752	144,529
106	CAN ALL INDUST	0	0	11,984	0	69
113	CAN Forestry and logging	509	2,797	0	144	7,548
115	CAN Agriculture and forestry activities	51	585	2,932	13	1,717
200	CAN Urban Primary Road Miles	1,874	82,882	3,491	284	10,848
210	CAN Rural Primary Road Miles	758	50,528	1,914	119	4,744

Code	Mexican or Canadian Surrogate Description	NH ₃	NO _x	PM _{2.5}	SO ₂	VOC
212	CAN Mining except oil and gas	0	0	3,536	0	0
220	CAN Urban Secondary Road Miles	3,506	126,804	6,784	603	26,809
221	CAN Total Mining	0	0	57,656	0	0
222	CAN Utilities	82	9,163	56,095	3,072	227
230	CAN Rural Secondary Road Miles	1,970	87,734	3,637	311	12,390
240	CAN Total Road Miles	45	67,129	2,442	73	107,438
308	CAN Food manufacturing	0	0	11,480	0	6,207
321	CAN Wood product manufacturing	306	1,980	0	161	8,202
323	CAN Printing and related support activities	0	0	0	0	11,919
324	CAN Petroleum and coal products manufacturing	0	1,089	1,376	433	6,561
326	CAN Plastics and rubber products manufacturing	0	0	0	0	22,854
327	CAN Non-metallic mineral product manufacturing	0	0	6,916	0	0
331	CAN Primary Metal Manufacturing	0	158	5,724	51	74
412	CAN Petroleum product wholesaler-distributors	0	0	0	0	40,364
448	CAN clothing and clothing accessories stores	0	0	0	0	118
562	CAN Waste management and remediation services	224	1,679	2,312	2,351	16,715
921	CAN Commercial Fuel Combustion	204	25,592	2,355	5,315	1,195
923	CAN TOTAL INSTITUTIONAL AND GOVERNEMNT	0	0	0	0	14,349
924	CAN Primary Industry	0	0	0	0	38,003
925	CAN Manufacturing and Assembly	0	0	0	0	72,660
926	CAN Distribtution and Retail (no petroleum)	0	0	0	0	7,168
927	CAN Commercial Services	0	0	0	0	31,818
932	CAN CANRAIL	56	100,494	2,396	354	5,080
941	CAN PAVED ROADS	0	0	315,987	0	0
945	CAN Commercial Marine Vessels	233	159,147	6,606	4,170	14,934
948	CAN Forest	0	21	7	0	236
950	CAN Combination of Forest and Dwelling	1,797	19,917	164,025	2,829	232,213
955	CAN UNPAVED ROADS AND TRAILS	0	0	477,941	0	0
960	CAN TOTBEEF	0	0	1,241	0	264,904
965	CAN TOTBEEF_CD	280,659	0	0	0	0
966	CAN TOTPOUL_CD	23,920	0	0	0	0
967	CAN TOTSWIN_CD	68,024	0	0	0	0
968	CAN TOTFERT_CD	120,207	0	0	0	0
970	CAN TOTPOUL	0	0	182	0	243
980	CAN TOTSWIN	0	0	757	0	2,591
990	CAN TOTFERT	0	3,743	380,161	9,570	150
996	CAN urban_area	0	0	1,305	0	0
1211	CAN Oil and Gas Extraction	2	35	240,377	149	937
1212	CAN OilSands	151	2,374	0	693	1,911
1251	CAN OFFR TOTFERT	111	106,004	7,733	81	10,726
1252	CAN OFFR MINES	44	38,370	3,312	32	4,174
1253	CAN OFFR Other Construction not Urban	27	21,854	3,747	20	9,680
1254	CAN OFFR Commercial Services	36	16,814	2,167	30	23,481
1255	CAN OFFR Oil Sands Mines	0	0	0	0	0
1256	CAN OFFR Wood industries CANVEC	14	10,922	1,089	10	1,995

Code	Mexican or Canadian Surrogate Description	NH ₃	NO _x	PM _{2.5}	SO ₂	VOC
1257	CAN OFFR Unpaved Roads Rural	35	9,857	1,756	30	69,379
1258	CAN OFFR Utilities	17	8,221	523	15	10,568
1259	CAN OFFR total dwelling	18	5,233	1,441	15	35,810
1260	CAN OFFR water	9	2,247	348	13	21,030
1261	CAN OFFR ALL INDUST	4	3,972	260	3	880
1262	CAN OFFR Oil and Gas Extraction	1	958	54	1	153
1263	CAN OFFR ALLROADS	2	1,015	74	1	523
1264	CAN OFFR OTHERJET	1	782	69	1	71
1265	CAN OFFR CANRAIL	0	77	8	0	14

3.5 Preparation of Emissions for the CAMx model

For this study, we perform air quality modeling with two models: CMAQ, and also the Comprehensive Air Quality Model with Extensions (CAMx model). Gridded hourly emissions output by the SMOKE model are used as emissions inputs to the CMAQ model, but they cannot be used directly as emissions inputs to the CAMx model. Instead, CMAQ-ready emissions must be converted to the format required by CAMx. The CAMx conversion process consists of the following:

- 1) Convert all emissions file formats from the I/O API NetCDF format used by CMAQ to the UAM format used by CAMx, including the merged, gridded low-level emissions files which include biogenics
- 2) Shift hourly emissions files from the 25 hour format used by CMAQ to the averaged 24 hour format used by CAMx
- 3) Rename and aggregate model species for CAMx
- 4) Convert 3D wildland and agricultural fire emissions into CAMx point format
- 5) Merge all inline point source emissions files together for each day, including layered fire emissions originally from SMOKE
- 6) Add sea salt aerosol emissions to the converted, gridded low-level emissions files

Conversion of file formats from I/O API to UAM is performed using a program called “cmaq2uam”. In the CAMx conversion process, all SMOKE outputs are passed through this step first. Unlike CMAQ, the CAMx model does not have an inline biogenics option, and so for the purposes of CAMx modeling, emissions from SMOKE must include biogenic emissions.

One difference between CMAQ-ready emissions files and CAMx-ready emissions files involves hourly temporalization. A daily emissions file for CMAQ includes data for 25 hours, where the first hour is 0:00 GMT of a given day, and the last hour is 0:00 GMT of the following day. For the CAMx model, a daily emissions file must only include data for 24 hours, not 25. Furthermore, to match the hourly configuration expected by CAMx, each set of consecutive hourly timesteps from CMAQ-ready emissions files must be averaged. For example, the first hour of a CAMx-ready emissions file will equal the average of the first two hours from the corresponding CMAQ-ready emissions file, and the last (24th) hour of a CAMx-ready emissions file will equal the average of the last two hours (24th and 25th) from the corresponding CMAQ-ready emissions file. This time conversion is incorporated into each step of the CAMx-ready emissions conversion process.

The CAMx model uses a slightly different version of the CB6 speciation mechanism than does the CMAQ model. SMOKE prepares emissions files for the CB6 mechanism used by the CMAQ model (“CB6-CMAQ”), and therefore, the emissions must be converted to the CB6 mechanism used by the CAMx model (“CB6-CAMx”) during the CAMx conversion process. In addition to the mechanism differences, CMAQ and CAMx also occasionally use different species naming conventions. For CAMx modeling, we also create additional tracer species. A summary of the differences between CMAQ input species and CAMx input species for CB6 (VOC), AE6 (PM_{2.5}), and other model species, is provided in Table 3-25. Each step of the CAMx-ready emissions conversion process includes conversion of CMAQ species to CAMx species using a species mapping table which includes the mappings in Table 3-25.

Table 3-25. Emission model species mappings for CMAQ and CAMx

Inventory Pollutant	CMAQ Model Species	CAMx Model Species
Cl ₂	CL2	CL2
HCl	HCL	HCL
CO	CO	CO
NO _x	NO	NO
	NO2	NO2
	HONO	HONO
SO ₂	SO2	SO2
	SULF	SULF
NH ₃	NH3	NH3
	NH3_FERT	n/a (not used in CAMx)
VOC	ACET	ACET
	ALD2	ALD2
	ALDX	ALDX
	BENZ	BENZ and BNZA (duplicate species)
	CH4	CH4
	ETH	ETH
	ETHA	ETHA
	ETHY	ETHY
	ETOH	ETOH
	FORM	FORM
	IOLE	IOLE
	ISOP	ISOP and ISP (duplicate species)
	KET	KET
	MEOH	MEOH
	NAPH + XYLMN (sum)	XYL
	NVOL	n/a (not used in CAMx)
	OLE	OLE
	PAR	PAR
	PRPA	PRPA
	SESQ	SQT
SOAALK	n/a (not used in CAMx)	
TERP	TERP and TRP (duplicate species)	
TOL	TOL and TOLA (duplicate species)	
UNR + NR (sum)	NR	
PM ₁₀	PMC	CPRM
PM _{2.5}	PEC	PEC
	PNO3	PNO3

Inventory Pollutant	CMAQ Model Species	CAMx Model Species
	POC	POC
	PSO4	PSO4
	PAL	PAL
	PCA	PCA
	PCL	PCL
	PFE	PFE
	PK	PK
	PH2O	PH2O
	PMG	PMG
	PMN	PMN
	PMOTHR	PMOTHR and FPRM (duplicate species)
	PNA	NA
	PNCOM	PNCOM
	PNH4	PNH4
	PSI	PSI
	PTI	PTI
	POC + PNCOM (sum)	POA ¹
	PAL + PCA + PFE + PMG + PK + PMN + PSI + PTI (sum)	FCRS ¹

¹ The POA species, which is the sum of POC and PNCOM, is passed to the CAMx model in addition to individual species POC and PNCOM. The FCRS species, which is also a sum of multiple PM species, is passed to CAMx in addition to each of the individual component species.

One feature which is part of CMAQ and is not part of CAMx involves plume rise for fires. For CMAQ modeling, we process fire emissions through SMOKE as inline point sources, and plume rise for fires is calculated within CMAQ using parameters from the inline emissions files (heat flux, etc). This is similar to how non-fire point sources are handled, except that the fire parameters are used to calculate plume rise instead of traditional stack parameters. The CAMx model supports inline plume rise calculations using traditional stack parameters, but, does not support inline plume rise for fire sources. Therefore, for the purposes of CAMx modeling, we must have SMOKE calculate plume rise for fires using the Laypoint program. In this modeling platform, this must be done for the ptfire, ptfire_othna, and ptagfire sectors. To distinguish these layered fire emissions from inline fire emissions, layered fire emissions are processed with the sector names “ptfire3D”, “ptfire_othna3D”, and “ptagfire3D”. When converting layered fire emissions files to CAMx format, stack parameters are added to the CAMx-ready fire emissions files to force the correct amount of fire emissions into each layer for each fire location.

CMAQ modeling uses one gridded low-level emissions file, plus multiple inline point source emissions files, per day. CAMx modeling also uses one gridded low-level emissions file per day - but instead of reading multiple inline point source emissions files at once, CAMx can only read a single point source file per day. Therefore, as part of the CAMx conversion process, all inline point source files are merged into a single “mrgpt” file per day. The mrgpt file includes the layered fire emissions described in the previous paragraph, in addition to all non-fire elevated point sources from the cmv_c3, othpt, ptegu, ptnonipm, and pt_oilgas sectors.

The remaining step in the CAMx emissions process is to generate sea salt aerosol emissions, which are distinct from the ocean chlorine emissions described in Section 2.8. Sea salt emissions do not need to be included in CMAQ-ready emissions because they are calculated by the model, but, do need to be included in CAMx-ready emissions. After the merged low-level emissions are converted to CAMx format, sea salt

emissions are generated using a program called “seasalt” and added to the low-level emissions. Sea salt emissions depend on meteorology, vary on a daily and hourly basis, and exist for model species PCL, NA, PSO4, and SS.

4 Emission Summaries

Table 4-1 summarizes emissions by sector for the 2016 alpha platform. This summary is provided at the national level by sector for the contiguous U.S. and for the portions of Canada and Mexico inside the larger 12km domain (12US1) discussed in Section 3.1. The afdust sector emissions represent the summaries *after* application of both the land use (transport fraction) and meteorological adjustments (see Section 2.2.1); therefore, this sector is called “afdust_adj” in these summaries. The onroad sector totals are post-SMOKE-MOVES totals, representing air quality model-ready emission totals, and include CARB emissions for California. The cmv sectors include U.S. emissions within state waters only; these extend to roughly 3-5 miles offshore and includes CMV emissions at U.S. ports. “Offshore” represents CMV emissions that are outside of U.S. state waters. Canadian CMV emissions are included in the other sector. The total of all sectors is listed as “Con U.S. Total.” State totals are available in the reports area on the FTP site for the 2016 alpha platform:

Table 4-1. National by-sector CAP emissions summaries for the 2016 alpha platform, 12US1 grid

Sector	CO	NH ₃	NO _x	PM ₁₀	PM _{2.5}	SO ₂	VOC
afdust adj	--	--	--	6,216,650	874,142	--	--
ag	--	2,776,552	--	--	--	--	179,970
cmv c1c2	47,183	120	260,338	6,493	6,168	345	4,840
cmv c3	10,885	25	108,268	4,248	3,832	3,883	5,043
nonpt	2,680,775	121,229	758,152	608,827	496,454	162,231	3,672,687
nonroad	12,188,930	2,266	1,206,980	122,107	115,409	2,418	1,464,613
np_oilgas	642,086	15	676,194	17,746	17,480	38,963	2,986,288
onroad	20,446,327	101,230	4,045,998	272,855	130,263	27,356	1,961,995
pt_oilgas	177,723	4,358	360,231	11,926	11,417	41,639	132,928
ptagfire	592,980	80,344	18,294	96,328	68,096	5,635	36,114
ptegu	672,184	25,012	1,289,229	170,818	140,823	1,544,799	33,453
ptfire	23,642,400	388,237	333,111	2,414,507	2,046,192	180,888	5,580,909
ptnonipm	1,847,809	61,395	1,072,555	407,458	263,816	672,952	808,939
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
Con U.S. Total	65,166,557	3,576,477	10,832,402	10,685,156	4,507,190	2,689,491	17,240,985
Canada othafdust	--	--	--	2,182,869	426,384	--	--
Canada othar	2,951,746	497,869	589,490	427,171	236,053	34,377	1,141,438
Canada onroad can	1,903,123	8,153	414,875	25,071	18,246	1,390	162,191
Canada othpt	1,147,803	18,699	600,674	90,358	48,248	869,280	790,253
Canada ptfire othna	761,707	13,036	16,385	84,528	71,778	6,733	185,609
Mexico othar	241,571	201,994	220,491	115,484	54,299	7,717	522,236
Mexico onroad_mex	1,828,101	2,789	442,410	15,151	10,836	6,247	158,812
Mexico othpt	205,081	5,049	447,645	73,252	57,437	476,077	71,030
Mexico ptfire othna	386,134	7,499	16,697	45,382	38,527	2,810	132,467
Offshore cmv_c1c2	56,548	184	284,208	9,219	8,942	224	5,263
Offshore cmv_c3	77,632	69	856,659	47,247	43,653	255,222	34,140
Offshore pt_oilgas	50,052	15	48,691	668	667	502	48,210
Non-US Total	9,609,498	755,356	3,938,226	3,116,400	1,015,070	1,660,580	3,251,647

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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

SCC	SCC description
2310020000	Industrial Processes;Oil and Gas Exploration and Production;Natural Gas;Total: All Processes
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

SCC	SCC description
2310021505	Industrial Processes;Oil and Gas Exploration and Production;On-Shore Gas Production;Fugitives: Valves
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

SCC	SCC description
2310023512	Industrial Processes;Oil and Gas Exploration and Production;Coal Bed Methane Natural Gas;Fugitives: Flanges
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 2016 alpha 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 profiles 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	PNC03_R	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	PNC03_R	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

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.

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 ₁ R ₂ >C=C<R ₃ R ₄)	4	Yes	Yes
KET	Ketone group (R ₁ R ₂ >C=O)	1	No (1 PAR)	Yes
OLE	Terminal olefin group (R ₁ R ₂ >C=C)	2	Yes	Yes
PAR	Paraffinic group (R ₁ -C<R ₂ R 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: <ul style="list-style-type: none"> 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 (-CEN).
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	<p>Guideline:</p> <ul style="list-style-type: none"> • 3 or less halogens – 1 PAR, 3 UNR • 4 or more halogens – 6 UNR <p>Examples:</p> <ul style="list-style-type: none"> • 1,3,5-Chlorobenzene – 1 PAR, 3 UNR • Tetrachlorobenzenes – 6 UNR
Cyclo dienes	<p>Guideline:</p> <ul style="list-style-type: none"> • 1 IOLE with additional carbons represented as alkyl groups (generally PAR) <p>Examples:</p> <ul style="list-style-type: none"> • Methylcyclopentadiene – 1 IOLE, 2 PAR • Methylcyclohexadiene – 1 IOLE, 3 PAR
Furans/Pyrroles	<p>Guideline:</p> <ul style="list-style-type: none"> • 2 OLE with additional carbons represented as alkyl groups (generally PAR) <p>Examples:</p> <ul style="list-style-type: none"> • 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	<p>Guideline:</p> <ul style="list-style-type: none"> • 1 OLE with remaining carbons represented as alkyl groups (generally PAR) <p>Examples:</p> <ul style="list-style-type: none"> • Ethylpyrazine – 1 OLE, 4 PAR • 1-methylpyrazole – 1 OLE, 2 PAR • 4,5-Dimethyloxazole – 1 OLE, 3 PAR
Triple bond(s)	<p>Guideline:</p> <ul style="list-style-type: none"> • 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. <p>Examples:</p> <ul style="list-style-type: none"> • 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 SPEICATEv4.5 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.

Appendix D: Mapping of Fuel Distribution SCCs to BTP, BPS and RBT

The table below provides a crosswalk between fuel distribution SCCs and classification type for portable fuel containers (PFC), fuel distribution operations associated with the bulk-plant-to-pump (BTP), refinery to bulk terminal (RBT) and bulk plant storage (BPS).

SCC	Type	Description
4030100 1	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Fixed Roof Tanks (Varying Sizes); Gasoline RVP 13: Breathing Loss (67000 Bbl. Tank Size)
4030100 2	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Fixed Roof Tanks (Varying Sizes); Gasoline RVP 10: Breathing Loss (67000 Bbl. Tank Size)
4030100 3	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Fixed Roof Tanks (Varying Sizes); Gasoline RVP 7: Breathing Loss (67000 Bbl. Tank Size)
4030100 4	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Fixed Roof Tanks (Varying Sizes); Gasoline RVP 13: Breathing Loss (250000 Bbl. Tank Size)
4030100 6	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Fixed Roof Tanks (Varying Sizes); Gasoline RVP 7: Breathing Loss (250000 Bbl. Tank Size)
4030100 7	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Fixed Roof Tanks (Varying Sizes); Gasoline RVP 13: Working Loss (Tank Diameter Independent)
4030110 1	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Floating Roof Tanks (Varying Sizes); Gasoline RVP 13: Standing Loss (67000 Bbl. Tank Size)
4030110 2	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Floating Roof Tanks (Varying Sizes); Gasoline RVP 10: Standing Loss (67000 Bbl. Tank Size)
4030110 3	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Floating Roof Tanks (Varying Sizes); Gasoline RVP 7: Standing Loss (67000 Bbl. Tank Size)
4030110 5	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Floating Roof Tanks (Varying Sizes); Gasoline RVP 10: Standing Loss (250000 Bbl. Tank Size)
4030115 1	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Floating Roof Tanks (Varying Sizes); Gasoline: Standing Loss - Internal
4030120 2	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Variable Vapor Space; Gasoline RVP 10: Filling Loss
4030120 3	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Variable Vapor Space; Gasoline RVP 7: Filling Loss
4040010 1	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Breathing Loss (67000 Bbl Capacity) - Fixed Roof Tank
4040010 2	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Breathing Loss (67000 Bbl Capacity) - Fixed Roof Tank
4040010 3	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Breathing Loss (67000 Bbl. Capacity) - Fixed Roof Tank
4040010 4	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Breathing Loss (250000 Bbl Capacity)-Fixed Roof Tank
4040010 5	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Breathing Loss (250000 Bbl Capacity)-Fixed Roof Tank
4040010 6	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Breathing Loss (250000 Bbl Capacity) - Fixed Roof Tank
4040010 7	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Working Loss (Diam. Independent) - Fixed Roof Tank
4040010 8	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Working Loss (Diameter Independent) - Fixed Roof Tank
4040010 9	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Working Loss (Diameter Independent) - Fixed Roof Tank
4040011 0	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Standing Loss (67000 Bbl Capacity)-Floating Roof Tank

SCC	Type	Description
4040011 1	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Standing Loss (67000 Bbl Capacity)-Floating Roof Tank
4040011 2	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Standing Loss (67000 Bbl Capacity)- Floating Roof Tank
4040011 3	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Standing Loss (250000 Bbl Cap.) - Floating Roof Tank
4040011 4	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Standing Loss (250000 Bbl Cap.) - Floating Roof Tank
4040011 5	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Standing Loss (250000 Bbl Cap.) - Floating Roof Tank
4040011 6	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13/10/7: Withdrawal Loss (67000 Bbl Cap.) - Float Rf Tnk
4040011 7	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13/10/7: Withdrawal Loss (250000 Bbl Cap.) - Float Rf Tnk
4040011 8	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Filling Loss (10500 Bbl Cap.) - Variable Vapor Space
4040011 9	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Filling Loss (10500 Bbl Cap.) - Variable Vapor Space
4040012 0	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Filling Loss (10500 Bbl Cap.) - Variable Vapor Space
4040013 0	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Specify Liquid: Standing Loss - External Floating Roof w/ Primary Seal
4040013 1	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Standing Loss - Ext. Floating Roof w/ Primary Seal
4040013 2	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Standing Loss - Ext. Floating Roof w/ Primary Seal
4040013 3	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Standing Loss - External Floating Roof w/ Primary Seal
4040014 0	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Specify Liquid: Standing Loss - Ext. Float Roof Tank w/ Secondary Seal
4040014 1	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Standing Loss - Ext. Floating Roof w/ Secondary Seal
4040014 2	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Standing Loss - Ext. Floating Roof w/ Secondary Seal
4040014 3	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Standing Loss - Ext. Floating Roof w/ Secondary Seal
4040014 8	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13/10/7: Withdrawal Loss - Ext. Float Roof (Pri/Sec Seal)
4040014 9	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Specify Liquid: External Floating Roof (Primary/Secondary Seal)
4040015 0	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Miscellaneous Losses/Leaks: Loading Racks
4040015 1	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Valves, Flanges, and Pumps
4040015 2	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Vapor Collection Losses
4040015 3	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Vapor Control Unit Losses
4040016 0	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Specify Liquid: Standing Loss - Internal Floating Roof w/ Primary Seal
4040016 1	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Standing Loss - Int. Floating Roof w/ Primary Seal
4040016 2	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Standing Loss - Int. Floating Roof w/ Primary Seal
4040016 3	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Standing Loss - Internal Floating Roof w/ Primary Seal

SCC	Type	Description
4040017 0	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Specify Liquid: Standing Loss - Int. Floating Roof w/ Secondary Seal
4040017 1	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Standing Loss - Int. Floating Roof w/ Secondary Seal
4040017 2	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Standing Loss - Int. Floating Roof w/ Secondary Seal
4040017 3	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Standing Loss - Int. Floating Roof w/ Secondary Seal
4040017 8	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13/10/7: Withdrawal Loss - Int. Float Roof (Pri/Sec Seal)
4040017 9	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Specify Liquid: Internal Floating Roof (Primary/Secondary Seal)
4040019 9	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; See Comment **
4040020 1	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 13: Breathing Loss (67000 Bbl Capacity) - Fixed Roof Tank
4040020 2	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 10: Breathing Loss (67000 Bbl Capacity) - Fixed Roof Tank
4040020 3	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 7: Breathing Loss (67000 Bbl. Capacity) - Fixed Roof Tank
4040020 4	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 13: Working Loss (67000 Bbl. Capacity) - Fixed Roof Tank
4040020 5	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 10: Working Loss (67000 Bbl. Capacity) - Fixed Roof Tank
4040020 6	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 7: Working Loss (67000 Bbl. Capacity) - Fixed Roof Tank
4040020 7	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 13: Standing Loss (67000 Bbl Cap.) - Floating Roof Tank
4040020 8	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 10: Standing Loss (67000 Bbl Cap.) - Floating Roof Tank
4040021 0	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 13/10/7: Withdrawal Loss (67000 Bbl Cap.) - Float Rf Tnk
4040021 1	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 13: Filling Loss (10500 Bbl Cap.) - Variable Vapor Space
4040021 2	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 10: Filling Loss (10500 Bbl Cap.) - Variable Vapor Space
4040021 3	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 7: Filling Loss (10500 Bbl Cap.) - Variable Vapor Space
4040023 0	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Specify Liquid: Standing Loss - External Floating Roof w/ Primary Seal
4040023 1	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 13: Standing Loss - Ext. Floating Roof w/ Primary Seal

SCC	Type	Description
4040023 2	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 10: Standing Loss - Ext. Floating Roof w/ Primary Seal
4040023 3	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 7: Standing Loss - External Floating Roof w/ Primary Seal
4040024 0	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Specify Liquid: Standing Loss - Ext. Floating Roof w/ Secondary Seal
4040024 1	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 13: Standing Loss - Ext. Floating Roof w/ Secondary Seal
4040024 8	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 10/13/7: Withdrawal Loss - Ext. Float Roof (Pri/Sec Seal)
4040024 9	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Specify Liquid: External Floating Roof (Primary/Secondary Seal)
4040025 0	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Loading Racks
4040025 1	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Valves, Flanges, and Pumps
4040025 2	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Miscellaneous Losses/Leaks: Vapor Collection Losses
4040025 3	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Miscellaneous Losses/Leaks: Vapor Control Unit Losses
4040026 0	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Specify Liquid: Standing Loss - Internal Floating Roof w/ Primary Seal
4040026 1	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 13: Standing Loss - Int. Floating Roof w/ Primary Seal
4040026 2	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 10: Standing Loss - Int. Floating Roof w/ Primary Seal
4040026 3	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 7: Standing Loss - Internal Floating Roof w/ Primary Seal
4040027 0	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Specify Liquid: Standing Loss - Int. Floating Roof w/ Secondary Seal
4040027 1	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 13: Standing Loss - Int. Floating Roof w/ Secondary Seal
4040027 2	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 10: Standing Loss - Int. Floating Roof w/ Secondary Seal
4040027 3	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 7: Standing Loss - Int. Floating Roof w/ Secondary Seal
4040027 8	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 10/13/7: Withdrawal Loss - Int. Float Roof (Pri/Sec Seal)

SCC	Type	Description
4040027 9	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Specify Liquid: Internal Floating Roof (Primary/Secondary Seal)
4040040 1	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Petroleum Products - Underground Tanks; Gasoline RVP 13: Breathing Loss
4040040 2	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Petroleum Products - Underground Tanks; Gasoline RVP 13: Working Loss
4040040 3	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Petroleum Products - Underground Tanks; Gasoline RVP 10: Breathing Loss
4040040 4	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Petroleum Products - Underground Tanks; Gasoline RVP 10: Working Loss
4040040 5	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Petroleum Products - Underground Tanks; Gasoline RVP 7: Breathing Loss
4040040 6	BTP/B PS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Petroleum Products - Underground Tanks; Gasoline RVP 7: Working Loss
4060010 1	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Splash Loading **
4060012 6	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Submerged Loading **
4060013 1	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Submerged Loading (Normal Service)
4060013 6	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Splash Loading (Normal Service)
4060014 1	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Submerged Loading (Balanced Service)
4060014 4	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Splash Loading (Balanced Service)
4060014 7	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Submerged Loading (Clean Tanks)
4060016 2	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Loaded with Fuel (Transit Losses)
4060016 3	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Return with Vapor (Transit Losses)
4060019 9	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Not Classified **
4060023 1	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Loading Tankers: Cleaned and Vapor Free Tanks
4060023 2	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Loading Tankers

SCC	Type	Description
4060023 3	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Loading Barges: Cleaned and Vapor Free Tanks
4060023 4	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Loading Tankers: Ballasted Tank
4060023 5	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Ocean Barges Loading - Ballasted Tank
4060023 6	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Loading Tankers: Uncleaned Tanks
4060023 7	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Ocean Barges Loading - Uncleaned Tanks
4060023 8	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Loading Barges: Uncleaned Tanks
4060023 9	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Tankers: Ballasted Tank
4060024 0	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Loading Barges: Average Tank Condition
4060024 1	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Tanker Ballasting
4060029 9	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Not Classified **
4060030 1	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Gasoline Retail Operations - Stage I; Splash Filling
4060030 2	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Gasoline Retail Operations - Stage I; Submerged Filling w/o Controls
4060030 5	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Gasoline Retail Operations - Stage I; Unloading **
4060030 6	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Gasoline Retail Operations - Stage I; Balanced Submerged Filling
4060030 7	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Gasoline Retail Operations - Stage I; Underground Tank Breathing and Emptying
4060039 9	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Gasoline Retail Operations - Stage I; Not Classified **
4060040 1	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Filling Vehicle Gas Tanks - Stage II; Vapor Loss w/o Controls
4060050 1	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Pipeline Petroleum Transport - General - All Products; Pipeline Leaks
4060050 2	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Pipeline Petroleum Transport - General - All Products; Pipeline Venting
4060050 3	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Pipeline Petroleum Transport - General - All Products; Pump Station
4060050 4	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Pipeline Petroleum Transport - General - All Products; Pump Station Leaks
4060060 2	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Consumer (Corporate) Fleet Refueling - Stage II; Liquid Spill Loss w/o Controls

SCC	Type	Description
4060070 1	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Consumer (Corporate) Fleet Refueling - Stage I; Splash Filling
4060070 2	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Consumer (Corporate) Fleet Refueling - Stage I; Submerged Filling w/o Controls
4060070 6	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Consumer (Corporate) Fleet Refueling - Stage I; Balanced Submerged Filling
4060070 7	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Consumer (Corporate) Fleet Refueling - Stage I; Underground Tank Breathing and Emptying
4068880 1	BTP/B PS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Fugitive Emissions; Specify in Comments Field
2501050 120	RBT	Storage and Transport; Petroleum and Petroleum Product Storage; Bulk Terminals: All Evaporative Losses; Gasoline
2501055 120	BTP/B PS	Storage and Transport; Petroleum and Petroleum Product Storage; Bulk Plants: All Evaporative Losses; Gasoline
2501060 050	BTP/B PS	Storage and Transport; Petroleum and Petroleum Product Storage; Gasoline Service Stations; Stage 1: Total
2501060 051	BTP/B PS	Storage and Transport; Petroleum and Petroleum Product Storage; Gasoline Service Stations; Stage 1: Submerged Filling
2501060 052	BTP/B PS	Storage and Transport; Petroleum and Petroleum Product Storage; Gasoline Service Stations; Stage 1: Splash Filling
2501060 053	BTP/B PS	Storage and Transport; Petroleum and Petroleum Product Storage; Gasoline Service Stations; Stage 1: Balanced Submerged Filling
2501060 200	BTP/B PS	Storage and Transport; Petroleum and Petroleum Product Storage; Gasoline Service Stations; Underground Tank: Total
2501060 201	BTP/B PS	Storage and Transport; Petroleum and Petroleum Product Storage; Gasoline Service Stations; Underground Tank: Breathing and Emptying
2501995 000	BTP/B PS	Storage and Transport; Petroleum and Petroleum Product Storage; All Storage Types: Working Loss; Total: All Products
2505000 120	RBT	Storage and Transport; Petroleum and Petroleum Product Transport; All Transport Types; Gasoline
2505020 120	RBT	Storage and Transport; Petroleum and Petroleum Product Transport; Marine Vessel; Gasoline
2505020 121	RBT	Storage and Transport; Petroleum and Petroleum Product Transport; Marine Vessel; Gasoline - Barge
2505030 120	BTP/B PS	Storage and Transport; Petroleum and Petroleum Product Transport; Truck; Gasoline
2505040 120	RBT	Storage and Transport; Petroleum and Petroleum Product Transport; Pipeline; Gasoline
2660000 000	BTP/B PS	Waste Disposal, Treatment, and Recovery; Leaking Underground Storage Tanks; Leaking Underground Storage Tanks; Total: All Storage Types

