Technical Support Document (TSD)

Preparation of Emissions Inventories for the Version 7.2

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
NH_3	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
PM_{10}	Particulate matter less than or equal to 10 microns
ppb, ppm	Parts per billion, parts per million
RBT	Refinery to Bulk Terminal
RFS2	Renewable Fuel Standard
RIA	Regulatory Impact Analysis

RICE	Reciprocating Internal Combustion Engine
RWC	Residential Wood Combustion
RPO	Regional Planning Organization
RVP	Reid Vapor Pressure
SCC	Source Classification Code
SESARM	Southeastern States Air Resource Managers
SESQ	Sesquiterpenes
SMARTFIRE	Satellite Mapping Automated Reanalysis Tool for Fire Incident Reconciliation
SMOKE	Sparse Matrix Operator Kernel Emissions
SO_2	Sulfur dioxide
SOA	Secondary Organic Aerosol
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
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 criteria air pollutants to represent the years of 2016 and 2028. The starting point for the 2016 inventory was the 2014 National Emissions Inventory (NEI), version 2 (2014NEIv2), although many inventory sectors were updated to represent the year 2016 through the incorporation of 2016-specific state and local data along with nationally-applied adjustment methods. The year 2028 inventory was developed starting with the 2016 inventory using sector-specific methods as described below.

The air quality modeling platform used for regional haze-related analyses 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 data and techniques including the emission inventories, the ancillary data files, and the approaches used to transform inventories for use in air quality modeling.

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. For the regional haze-related emissions modeling documented in this TSD, the emissions values for most sectors are the same as those in the Inventory Collaborative 2016beta Emissions Modeling Platform, available from http://views.cira.colostate.edu/wiki/wiki/10197. The specification sheets posted on the 2016beta platform release page provide many details regarding the inventories and emissions modeling techniques in addition to those addressed in this TSD.

This 2016 emissions modeling platform includes all criteria air pollutants (CAPs) and precursors, and a group of hazardous air pollutants (HAPs). 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 modeling domain includes the lower 48 states and parts of Canada and Mexico. The modeling cases for this platform were developed for the Comprehensive Air Quality Model with Extensions (CAMx). However, the emissions modeling process first prepares outputs in the format used by CMAQ, after which those emissions data are converted to the formats needed by CAMx.

The 2016 platform used in this study consists of a 2016 base case and a 2028 case with the abbreviations **2016fg_16j** and **2028fg_16j**, respectively. An additional 2028 case that included source apportionment by inventory sector named **2028fg_secsa_16j** was also developed. This platform accounts for atmospheric chemistry and transport within a state of the art photochemical grid model. In the case abbreviation 2016fg_16j, 2016 is the year represented by the emissions; the "f" represents the base year emissions modeling platform iteration, which here shows that it is 2014NEI-based (whereas for 2011 NEI-based platforms, this letter was "e"); and the "g" stands for the seventh configuration of emissions modeled for a 2014-NEI based modeling platform.

The platform includes point sources, nonpoint sources, commercial marine vessels (CMV), onroad and nonroad mobile sources, and fires for the U.S., Canada, and Mexico. 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 modeling platform and the NEI are developed using the same inputs, but the NEI emissions are aggregated to vehicle type/fuel type totals and annual temporal resolution while the platform emissions have more finely resolved SCCs and temporal resolution. Temporal, spatial and other changes in emissions between the NEI and the emissions input into the platform are described primarily in the beta platform specification sheets. Emissions from Canada and Mexico are used for the platform but are not part of the NEI.

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 4.6 (SMOKE 4.6[2]) with some updates. Emissions files were created for a 36-km national grid and for a 12-km national grid, both of which include 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 (GHRSST) (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 "2016fg_16j."

This document contains five sections and several appendices. Section 2 describes the 2016 and 2028 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] It was determined after the modeling for this study was complete that a library used by SMOKE 4.6 was not initializing the earth ellipsoid to match the spherical earth that is used for the air quality modeling as it had in previous versions. This could result in shifting of the locations for point sources to change by up to about 1-km, which in some cases could change the specific grid cell assigned to the source. The total emission would not change, only the modeling grid cell assigned for some sources. If further studies are performed with emission inputs from this study, EPA results can be reproduced using the version of SMOKE provided with the beta platform. If studies are not concerned with reproducing the EPA results, it is recommended that SMOKE 4.7 be used which corrects this issue.

2 Emission Inventories and Approaches

This section summarizes the year 2016 and 2028 emissions data that make up the regional haze platform. This section provides details about the data contained in each of the platform sectors for the base year and the future year. Differences between the 2016 beta platform and the regional haze platform are also discussed.

2.1 Summary of 2016 Base Year Emission Inventories

The starting point for many emission inputs is the 2014NEIv2 although in some cases with more detailed temporal/spatial resolution data, although the emissions have been updated to better represent the year 2016. 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. In addition to the NEI-based data for the broad categories of point, nonpoint, onroad, nonroad, and events (i.e., fires), emissions from the Canadian and Mexican inventories and several other non-NEI data sources are included in the 2016 platform.

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 collaborates extensively with S/L/T agencies to ensure a high quality of data in the NEI. Using the 2014NEIv2 as a starting point, the National Inventory Collaborative worked to develop a modeling platform that more closely represents the year 2016. All emissions modeling sectors were modified in some way to better represent the year 2016 for the beta platform, which was slightly adjusted to prepare the regional haze platform used in this study. In terms of emissions totals, only the Canadian fugitive dust emissions differ from those in the beta platform.

The point source emission inventories for the platform include partially updated emissions for 2016. Agricultural and wildland fire emissions represent the year 2016. Most nonpoint source sectors started with 2014NEIv2 emissions and were adjusted to better represent the year 2016. Fertilizer emissions, nonpoint oil and gas emissions, and onroad and nonroad mobile source emissions represent the year 2016. For commercial marine vessel (CMV) emissions, SO_2 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. Nonpoint oil and gas emissions were developed using 2016-specific data for oil and gas wells and their 2016 production levels.

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 nationally available data sets. Onroad emissions for the platform were developed based on emissions factors output from MOVES2014a for the year 2016, run with inputs derived from the 2014NEIv2 including activity data (e.g., vehicle miles traveled and vehicle populations) projected to the year 2016. MOVES2014b was used to generate nonroad emissions because it included important updates related to nonroad engine population growth rates.

For the purposes of preparing the air quality model-ready emissions, emissions from the five NEI data categories are 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. For studies that use CAMx, these CMAQ-ready emissions inputs are then converted into the formats needed by CAMx.

Table 2-1 presents an overview the sectors in the 2016 platform and how they generally relate to the 2014NEIv2 as their 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. Through the Collaborative workgroups, state and local agencies provided data used in the development of most sectors.

Table 2-1. Platform sectors for the 2016 regional haze emissions modeling case

Platform Sector: *abbreviation*	**NEI Data Category**	**Description and resolution of the data input to SMOKE**
EGU units: *Ptegu*	Point	Point source electric generating units (EGUs) for 2016 from the Emissions Inventory System (EIS), based on 2014NEIv2 with some sources updated to 2016. Includes some specific S/L updates. 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: *pt_oilgas*	Point	Point sources for 2016 including S/L updates for 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 year 2016 in the baseline inventory were projected from 2014 to 2016. Annual resolution.
Remaining non-EGU point: *Ptnonipm*	Point	All 2016 point source inventory records not matched to the ptegu or pt_oilgas sector, including updates submitted by state and local agencies. Aircraft and airport ground support emissions not submitted for 2016 were adjusted to year 2016 using FAA data. Year 2016 rail yard emissions were developed by the rail workgroup. Annual resolution.
Agricultural: *Ag*	Nonpoint	Nonpoint livestock and fertilizer application emissions. Livestock includes ammonia and other pollutants (except PM2.5) and was projected from 2014NEIv2 based on animal population data from the U.S. Department of Agriculture (USDA) National Agriculture Statistics Service Quick Stats, where available. Fertilizer includes only ammonia and is estimated for 2016 using the FEST-C model. County and monthly resolution.
Agricultural fires with point resolution: *ptagfire*	Nonpoint	2016 agricultural fire sources based on EPA-developed data with state updates, represented as point source day-specific emissions. They are in the nonpoint NEI data category, but in the platform, they are treated as point sources. Mostly at daily resolution with some state-submitted data at monthly resolution.

Platform Sector: *abbreviation*	NEI Data Category	Description and resolution of the data input to SMOKE
Area fugitive dust: ***Afdust***	Nonpoint	PM_{10} and $PM_{2.5}$ fugitive dust sources from the 2014NEIv2 nonpoint inventory with paved road dust grown to 2016 levels; including building construction, road construction, agricultural dust, and road dust. The NEI emissions are reduced during modeling according to a transport fraction (newly computed for the beta platform) and a meteorology-based (precipitation and snow/ice cover) zero-out. County and annual resolution.
Biogenic: ***Beis***	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 "water fix" land use data (including improved treatment of water grid cells).
Category 1, 2 CMV: ***cmv_c1c2***	Nonpoint	Category 1 (C1) and category 2 (C2) commercial marine vessel (CMV) emissions sources projected to 2016 from the 2014NEIv2 nonpoint inventory based on factors from the Regulatory Impact Analysis (RIA) Control of Emissions of Air Pollution from Locomotive Engines and Marine Compression Ignition Engines Less than 30 Liters per Cylinder[3]. County and annual resolution.
Category 3 CMV: ***cmv_c3***	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. Emissions are projected to 2016 from 2014NEIv2 based on factors derived from U.S. Army Corps of Engineers Entrance and Clearance data and information about the ships entering the ports.
Locomotives: ***rail***	Nonpoint	Rail locomotives emissions developed by the rail workgroup based on 2016 activity and emission factors. Includes freight and commuter rail emissions and incorporates state and local feedback. County and annual resolution.
Remaining nonpoint: ***nonpt***	Nonpoint	2014NEIv2 nonpoint sources not included in other platform sectors with sources proportional to human population activity data grown to year 2016; incorporates state and local feedback. County and annual resolution.
Nonpoint source oil and gas: ***np_oilgas***	Nonpoint	2016 nonpoint oil and gas emissions output from the NEI oil and gas tool along with state and local feedback. County and annual resolution.
Residential Wood Combustion: ***rwc***	Nonpoint	2014NEIv2 nonpoint sources from residential wood combustion (RWC) processes projected to the year 2016. County and annual resolution.
Nonroad: ***nonroad***	Nonroad	2016 nonroad equipment emissions developed with the MOVES2014b model which incorporates updated equipment growth rates. MOVES was used for all states except California, which submitted emissions. County and monthly resolution.

[3] https://nepis.epa.gov/Exe/ZyPDF.cgi/P10023S4.PDF?Dockey=P10023S4.PDF

Platform Sector: *abbreviation*	NEI Data Category	Description and resolution of the data input to SMOKE
Onroad: ***onroad***	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 coupled with activity data projected to year 2016 or provided by S/Ls. SMOKE-MOVES was used to compute emissions from the emission factors and activity data.
Onroad California: ***onroad_ca_adj***	Onroad	2016 California-provided CAP onroad mobile source gasoline and diesel vehicles based on the EMFAC model, which ere gridded and temporalized using MOVES2014a results. Volatile organic compound (VOC) HAP emissions derived from California-provided VOC emissions and MOVES-based speciation.
Point source fires- ***ptfire***	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). Incorporates state inputs. Daily resolution.
Non-US. fires: ***ptfire_othna***	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). Daily resolution.
Other Area Fugitive dust sources not from the NEI: ***othafdust***	N/A	Fugitive dust sources of particulate matter emissions excluding land tilling from agricultural activities, from Environment and Climate Change Canada (ECCC) 2015 emission inventory, except that for regional haze, construction dust emissions were reduced to levels compatible with their 2010 inventory. 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 Fugitive dust sources not from the NEI: ***othptdust***	N/A	Fugitive dust sources of particulate matter emissions from land tilling from agricultural activities, from Environment and Climate Change Canada (ECCC) 2015 emission inventory, but for regional haze wind erosion emissions were removed. A transport fraction adjustment is applied along with a meteorology-based (precipitation and snow/ice cover) zero-out. Data were originally provided on a rotated 10-km grid for beta, but were smoothed for regional so as to avoid the artifact of grid lines in the processed emissions. Monthly resolution.
Other point sources not from the NEI: ***othpt***	N/A	Point sources from the ECCC 2015 emission inventory, including agricultural ammonia, along with emissions from Mexico's 2008 inventory projected to 2014 and 2018 and then interpolated to 2016. Agricultural data were originally provided on a rotated 10-km grid for beta, but were smoothed for regional so as to avoid the artifact of grid lines in the processed emissions. Monthly resolution for Canada agricultural and airport emissions, annual resolution for the remainder of Canada and all of Mexico.

Platform Sector: *abbreviation*	NEI Data Category	Description and resolution of the data input to SMOKE
Other non-NEI nonpoint and nonroad: ***othar***	N/A	Year 2015 Canada (province or sub-province resolution) emissions from the ECCC inventory: monthly for nonroad sources; annual for rail, CMV and other nonpoint Canada sectors. Year 2016 Mexico (municipio resolution) emissions, interpolated from 2014 and 2018 inventories that were projected from their 2008 inventory: annual nonpoint and nonroad mobile inventories.
Other non-NEI onroad sources: ***onroad_can***	N/A	Monthly year 2015 Canada (province resolution or sub-province resolution, depending on the province) from the ECCC onroad mobile inventory. Also includes onroad emissions in Alaska, Hawaii, Puerto Rico, and Virgin Islands from 2014NEIv2.
Other non-NEI onroad sources: ***onroad_mex***	N/A	Monthly year 2016 Mexico (municipio resolution) onroad mobile inventory based on MOVES-Mexico runs for 2014 and 2018 then interpolated to 2016.

Other natural emissions are also merged in with the above sectors: ocean chlorine and sea salt. 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). In CMAQ, the species name is "CL2". The sea salt emissions were developed with version 4.1 of the OCEANIC pre-processor that comes with the CAMx model. The preprocessor estimates time/space-varying emissions of aerosol sodium, chloride and sulfate; gas-phase chlorine and bromine associated with sea salt; gaseous halo-methanes; and dimethyl sulfide (DMS). These additional oceanic emissions are incorporated into the final model-ready emissions files for CAMx.

The emission inventories in SMOKE input formats for the regional haze platform are available from 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 "2016v7.2 (beta and regional haze) Platform". The 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. Additional types of data including outputs from SMOKE and inputs to CAMx will be available from the Intermountain West Data Warehouse.

2.2 Inventory Differences from the 2016 beta platform

This section describes how the regional haze cases differ from the 2016 beta platform case 2016ff. Note that most of the emissions updates are spatial allocation changes only and do not change the emissions totals that would be seen in summaries, although the dust emissions in Canada were lowered.

2.2.1 Prescribed Fires Spatial Reallocation

Prescribed fire data were submitted for the beta platform by certain states, and in these data some Kansas (Flint Hills grasslands) and Georgia prescribed fire emissions were located at county centroids, which was not realistic. These issues are illustrated in Figure 2-1. For the regional haze platform, these emissions were re-gridded to spread the emissions out to other parts of each county. The emissions were placed in areas with appropriate types of land use for these types of fires: 2011 National Land Cover Database (NLCD) forest land in Georgia and 2011 NLCD grass-land in Kansas. Note that the total of these emissions did not change as a result of the regridding process – only the spatial allocation. Examples of fires before and after the spatial reallocation are shown in Figures 2-1 through 2-6. 2016 annual wildland fires are shown in Figure 2-7 for reference.

In addition, to support 36/12km two-way nesting with CAMx that was used for this study, the gridded 36km and 12km point source prescribed fire emissions file had to be combined to use the appropriate resolution in each area of the grid. This issue only affects 2-way nested CAMx model runs and is described further in Section 3.5.2.

Figure 2-1. National wildland and prescribed fires for 2016 beta (March 2016, short tons)

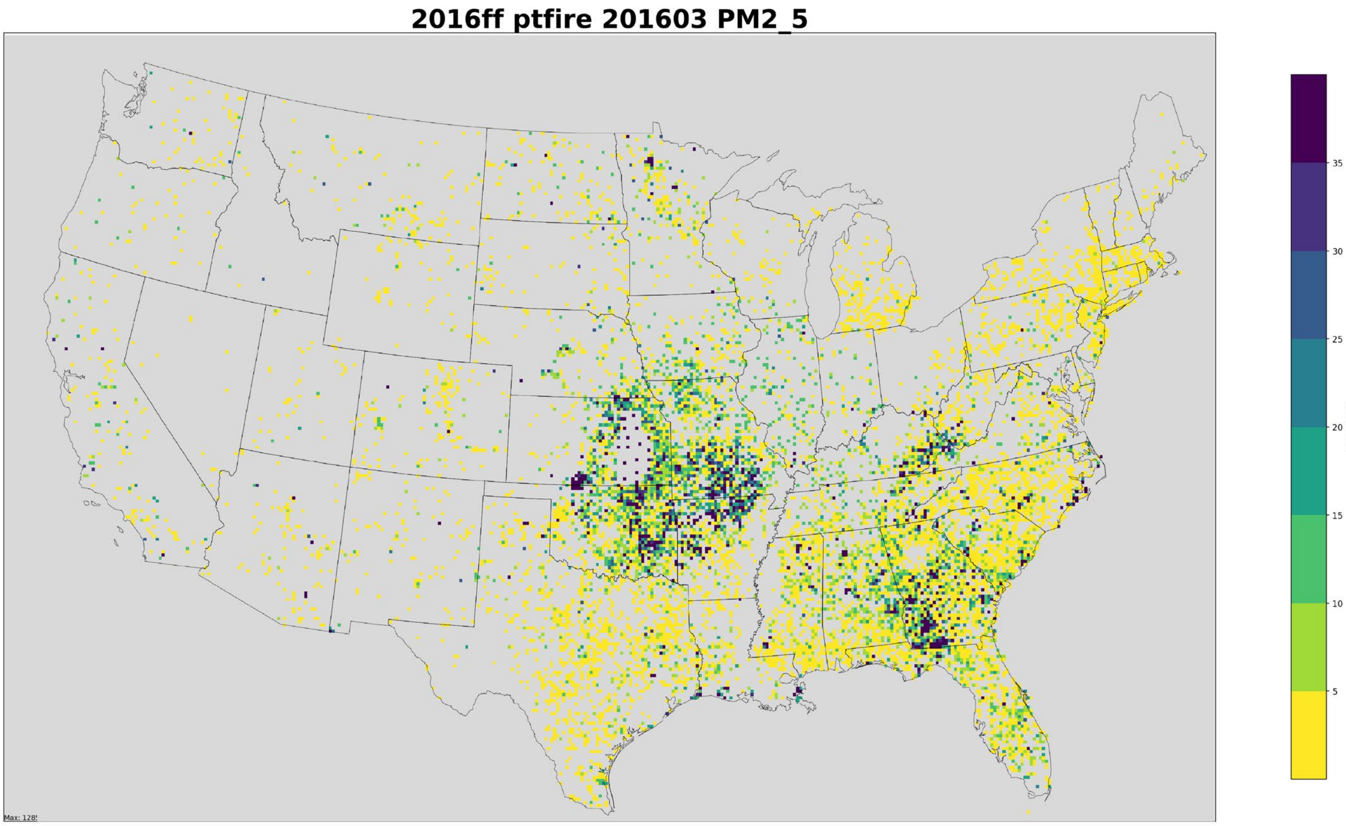


Figure 2-2. Georgia Prescribed Fire Emissions Concentrated at County Centroids

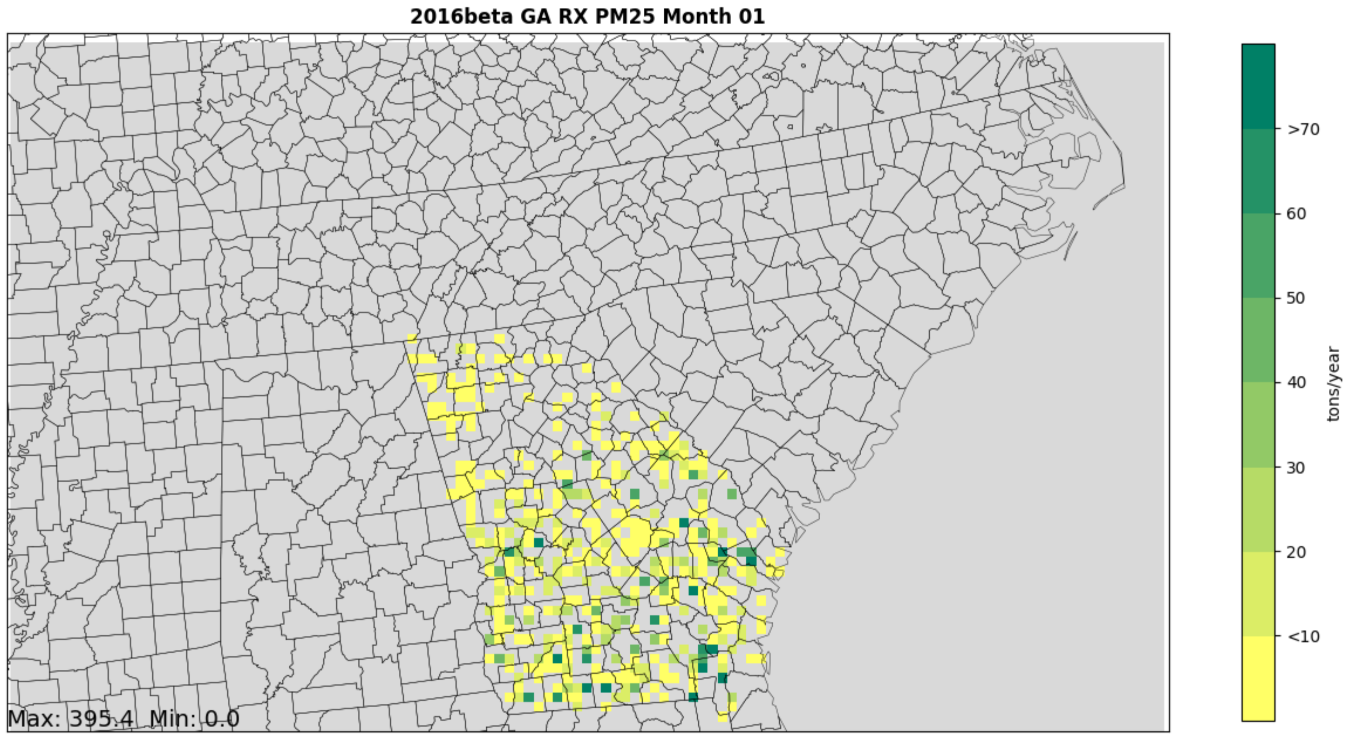


Figure 2-3. Georgia Prescribed Fire Emissions after re-gridding

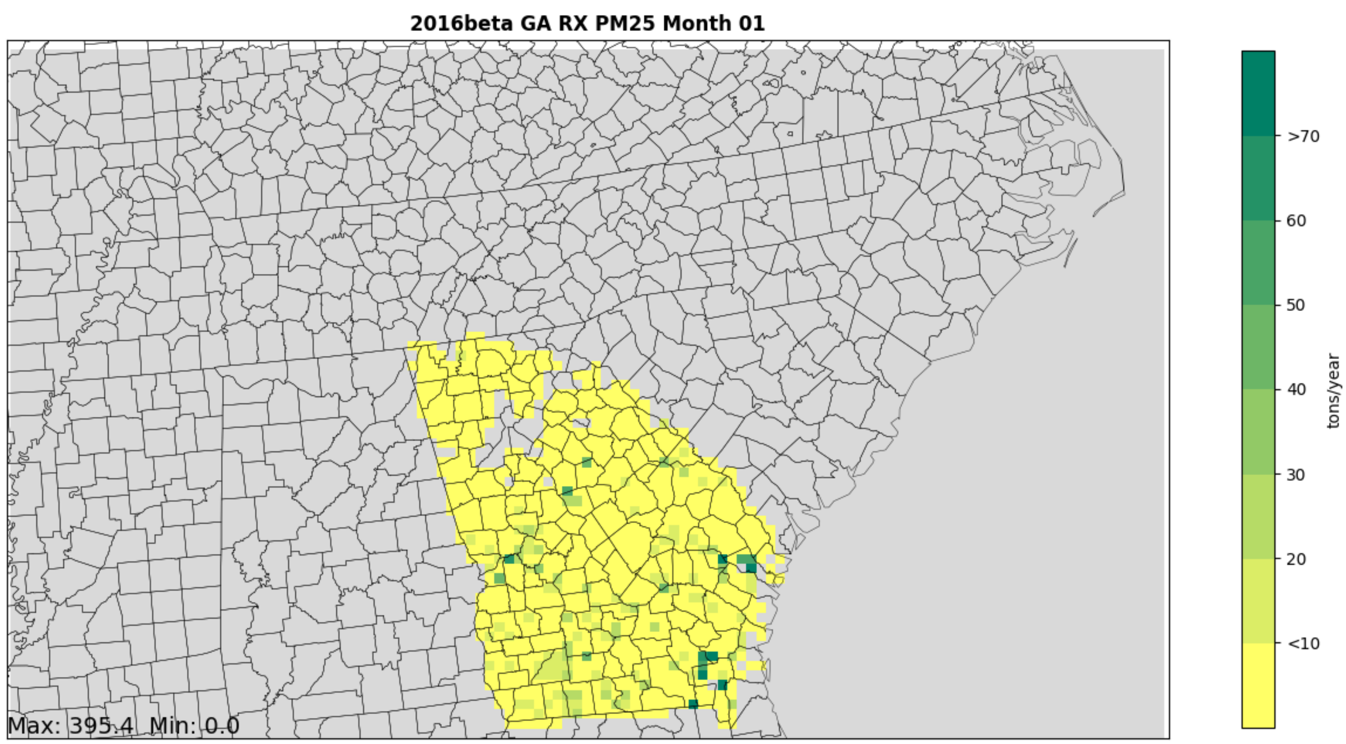


Figure 2-4. Kansas Prescribed Fire Emissions Concentrated at County Centroids

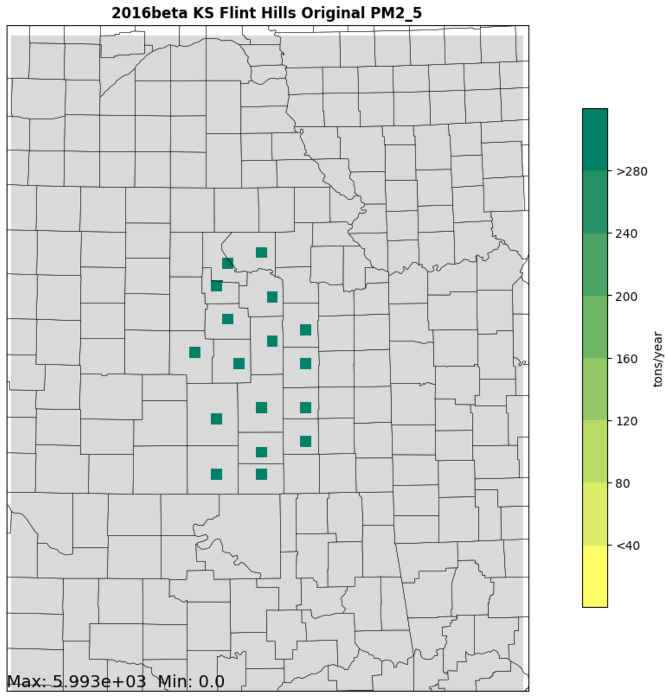


Figure 2-5. Kansas Prescribed Fire Emissions after re-gridding

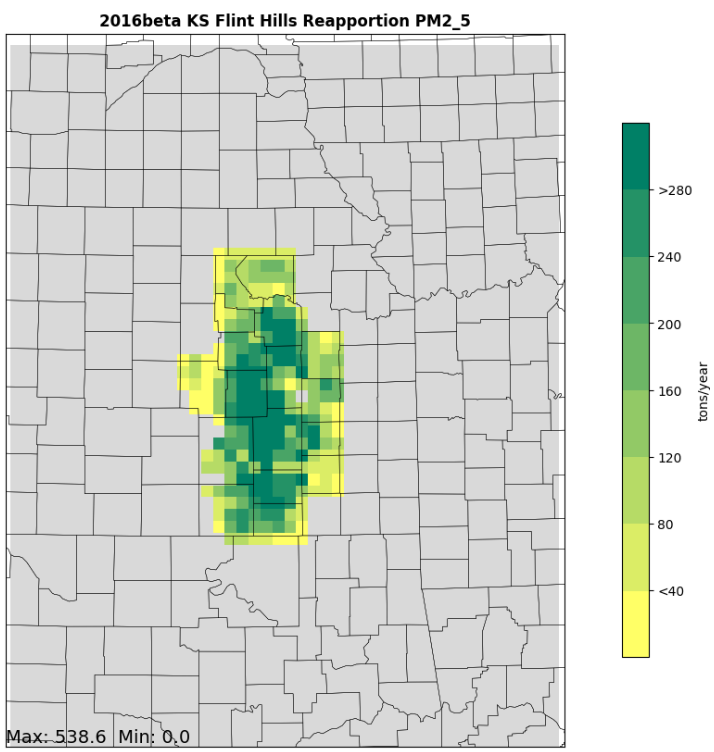


Figure 2-6. Corrected annual prescribed fires for 2016 regional haze

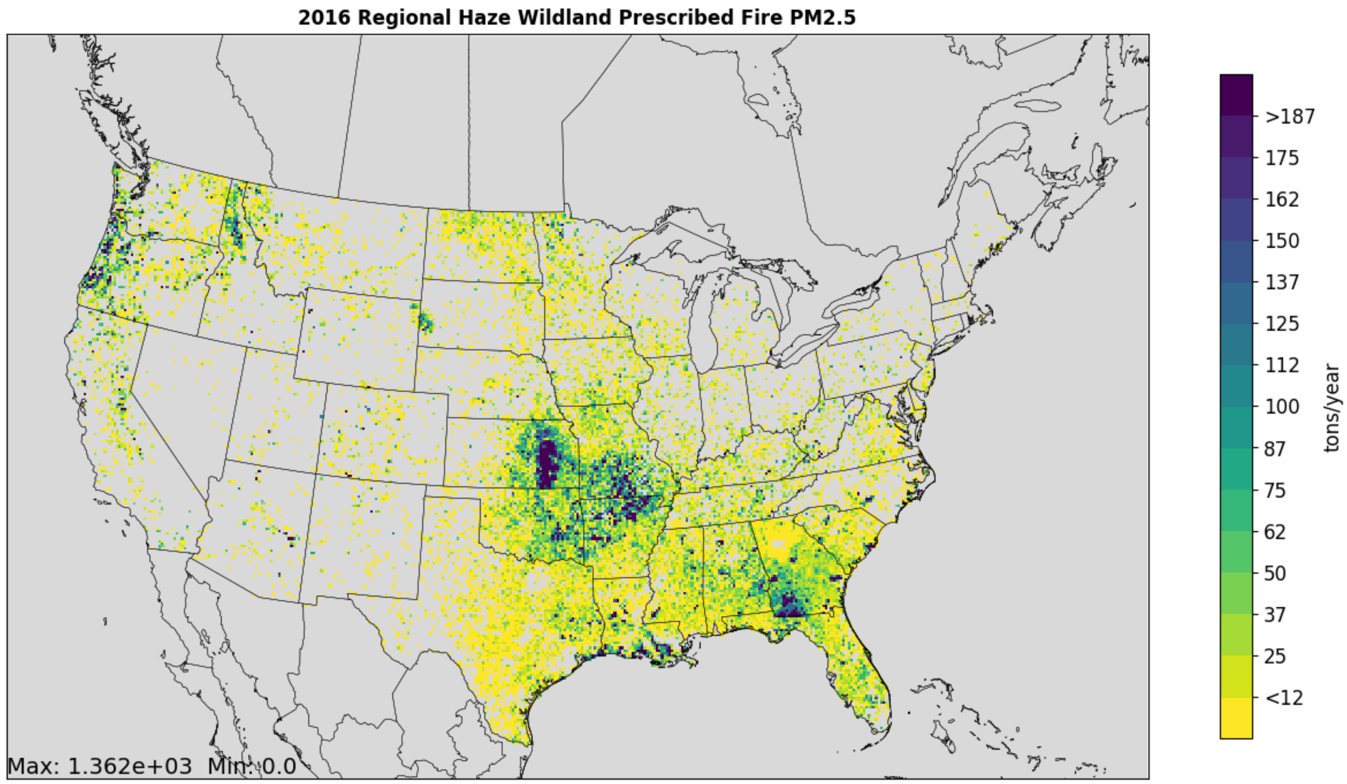
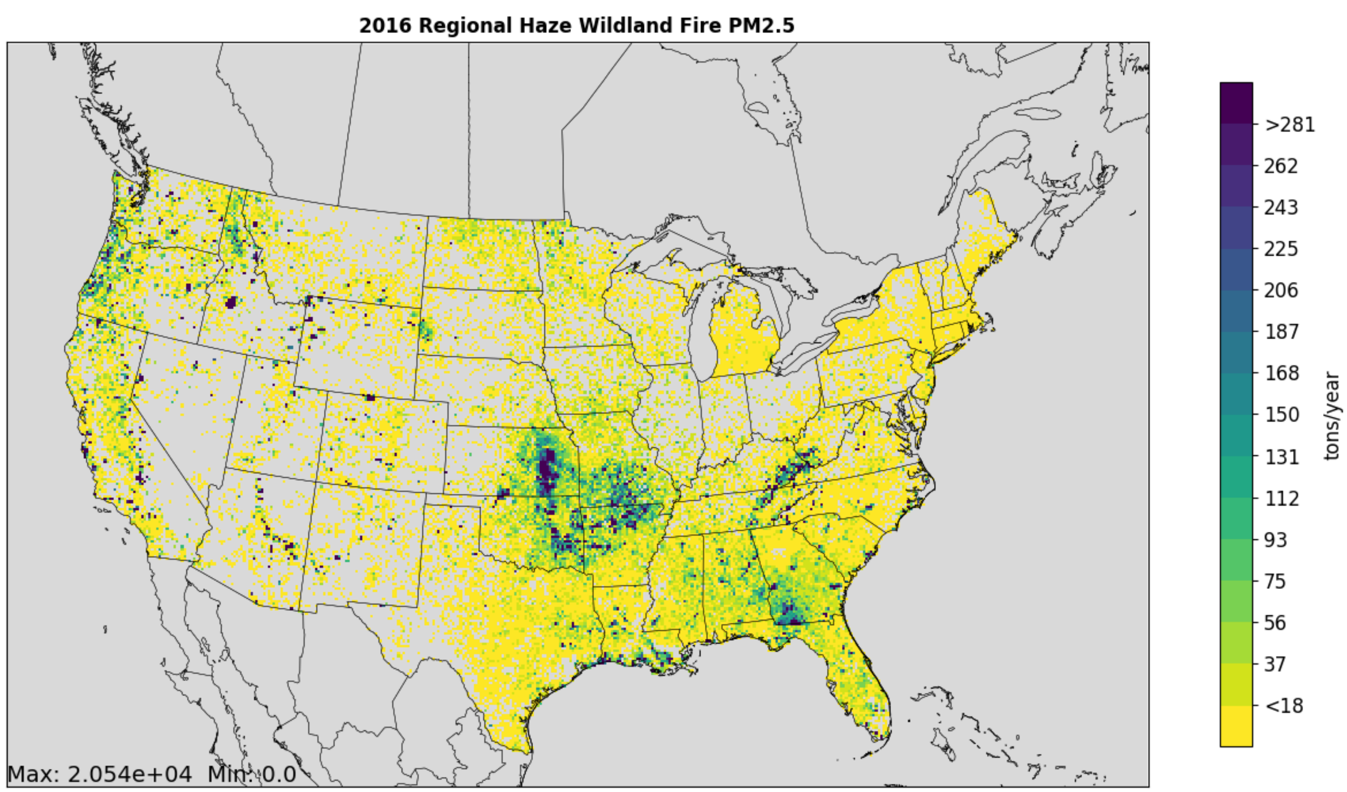


Figure 2-7. Wildland fires for 2016 regional haze



2.2.2 Adjustments to Canadian Emissions

In the 2016ff (beta) model run, very high modeled "soil particulate matter (PM)" concentrations were noted in the spring in Alberta and Saskatchewan. ECCC confirmed that they had also seen this issue and had adjusted some of their dust emission categories downward as a result of the modeled PM being high compared to monitors in the area. They noted that the emissions inventory method for these emissions had changed in recent inventories. To reduce this issue of high PM, adjustments to construction dust were made to make those more consistent with the ECCC 2010 inventory, and wind erosion dust was removed because this category is not included in the US emissions.

In addition, several categories of agricultural Canadian emissions were received in a gridded format. Since the Canadian grids and the EPA grids did not match, a "waffle" pattern was observed in some of the EPA gridded data. EPA re-gridded the raw Canadian data to reflect the EPA 36km and 12km grids without the waffling. The pattern in the original beta platform and an example of the regridded data are shown in Figure 2-5 and Figure 2-6, respectively (note that the plots are on different scales). More specifically, spatial apportionment factors were calculated using the area of overlap between the 10 km Canada Lambert grid and a 4 km resolution grid with the same boundaries and grid projection as the 36US3 modeling domain. The 2015 Canada point dust emissions were placed into the 10 km grid cells based on the inventory latitude and longitude and aggregated by province and location. The spatial factors were then applied to allocate the emissions to the 4 km grid cells. Centroid latitude and longitudes for each respective emitting 4 km grid cell were used to fill the location information of the resulting point Flat File. The 4 km resolution inventories were then aggregated to 12 km resolution in order to reduce the size of the inventory.

Figure 2-8. Example of gridding artifact that existed in some Canadian emissions in 2016 beta

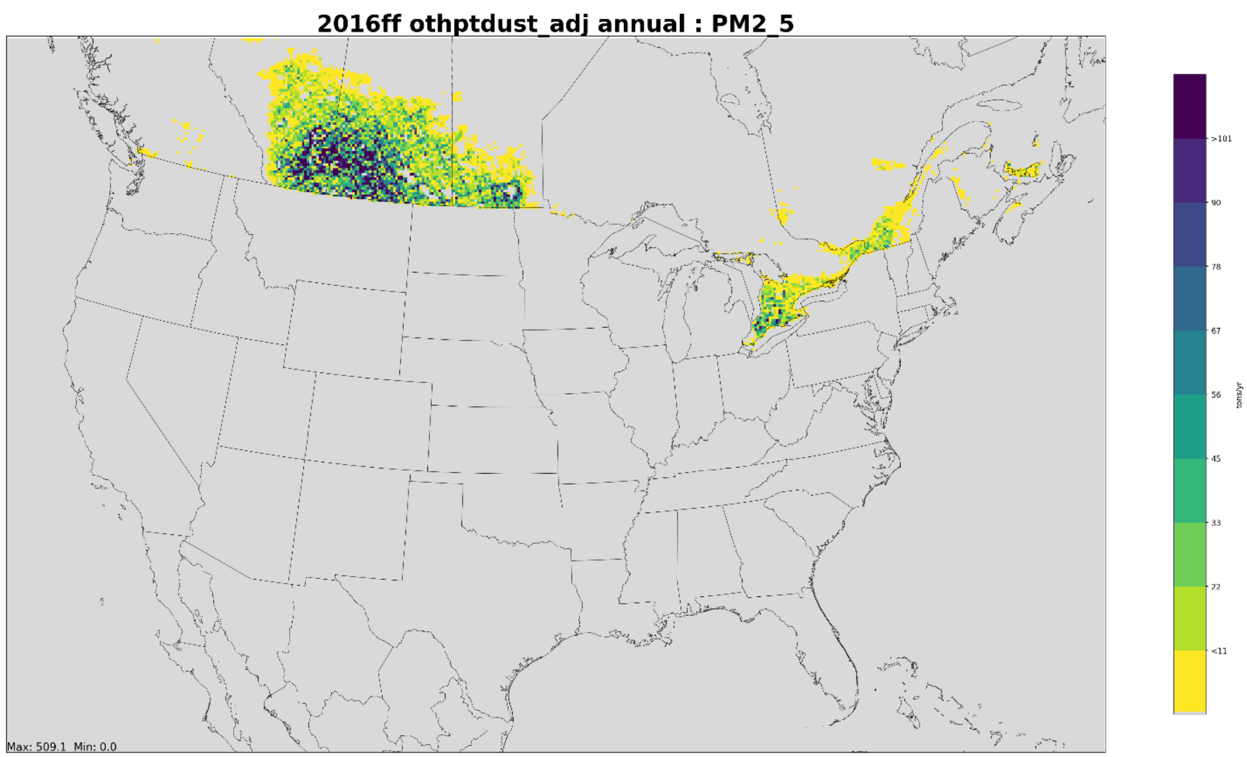
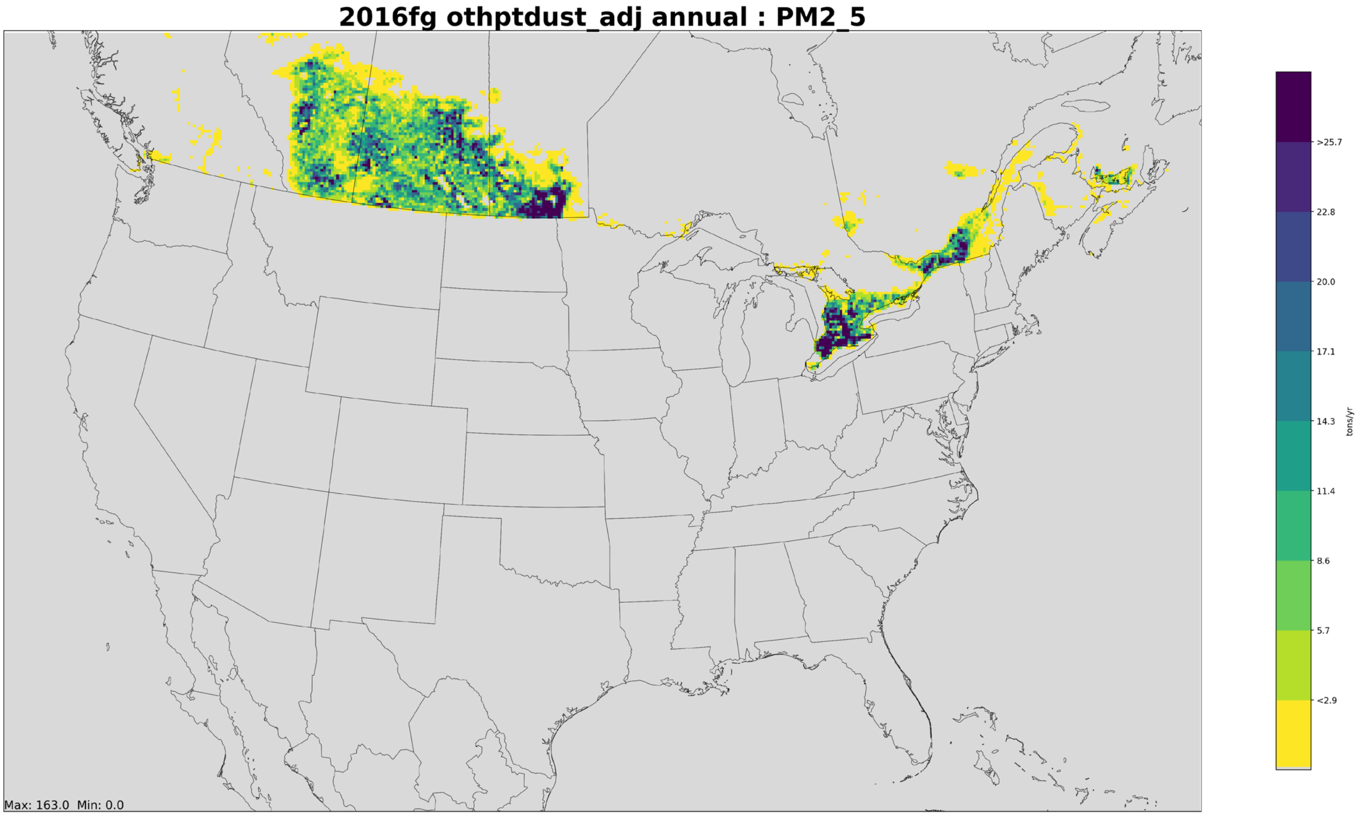


Figure 2-9. Emissions after the gridding artifact was removed



2.2.3 Moving sources from ptnonipm to ptegu and other EGU refinements

Following the 2016ff (aka beta) modeling, some sources in the ptnonipm inventory were found in an output from the Integrated Planning Model (IPM), which is a model used to estimate future year EGU emissions.. As a result, they were matched to the sources in the database that is input to IPM and were moved from ptnonipm to ptegu sector. If the sources were left in the ptnonipm inventory they would be double-counted with emissions output from IPM when modeling future years. The units moved from ptnonipm to ptegu are listed in Table 2-2. In addition, a newer version of SMOKE was used to process emissions for the regional haze case that corrects cases when CEMS data have NOx missing for the entire year. This is important in certain areas for the base year, such as a source in Utah, and more so in future year cases.

Table 2-2. Units moved from ptnoipm to ptegu in the regional haze cases

EIS Facility ID	EIS Unit ID	NEEDS ID	ORIS Facility Code	ORIS Boiler ID
5783911	119254913	50837_B_UNIT1	50837	UNIT1
5783911	119255013	50837_B_UNIT2	50837	UNIT2
533611	91819113	57898_B_BLR3	57898	BLR3
533611	91819213	57898_B_BLR4	57898	BLR4
533611	91819313	57898_B_BLR5	57898	BLR5
7869811	87378813	50878_B_UNIT1	50878	UNIT1

EIS Facility ID	EIS Unit ID	NEEDS ID	ORIS Facility Code	ORIS Boiler ID
8057311	112375613	50630_B_BLR1	50630	BLR1
8057311	112375613	50630_B_BLR2	50630	BLR2
3109711	124523513	59254_G_GENS1	59254	GENS1
4837411	90282913	3456_G_5CA1	3456	5CA1
12807411	123689413	54775_B_BLR10	54775	BLR10
12807411	123689013	54775_B_BLR11	54775	BLR11
7663611	12450313	58205_B_1	B	1
6719911	12840813	56119_G_300	56119	300
5632711	69997613	56152_G_CTG1	56152	CTG1
5633011	20889913	10167_G_GEN1	10167	GEN1
6940911	14044213	55596_G_0001	55596	0001
6940911	124476513	55596_G_0002	55596	0002
6940911	124476613	55596_G_0003	55596	0003
6940911	82780713	55596_G_0004	55596	0004

2.3 Summary of 2028 Future Year Emission Inventories

This section describes how the 2028 future year emissions inventories were developed for the 2016 beta and regional haze platforms. For the 2028 modeling, emissions for some sectors were kept the same as those used in the 2016 air quality modeling, while others were projected to future year levels that represent 2028. Emissions for the following sectors are the same for the base and future year: beis, ptagfire, ptfire, ptfire_othna, ocean_cl2, and sea salt. All remaining sectors have been projected to 2028 as summarized in Table 2-3. Additional information regarding the projection techniques applied to each sector can be found in the 2016 beta platform specification sheets.

Table 2-3. Overview of projection methods for the 2028 regional haze cases

Platform Sector: *abbreviation*	**Description of Projection Method for regional haze case**
EGU units: *Ptegu*	The Integrated Planning Model (IPM) was run to create the 2028 emissions. The 2030 model output year from the November, 2018 version of the IPM platform was used (https://www.epa.gov/airmarkets/power-sector-modeling-platform-v6-november-2018). Emission inventory Flat Files for input to SMOKE were generated using post-processed IPM output data. Temporal allocation for future year emissions is discussed in the EGU-IPM specification sheet for the 2016 beta platform.
Point source oil and gas: *pt_oilgas*	First, known closures were applied to the 2016 pt_oilgas sources. Production-related sources were then grown from 2016 to 2017 using historic production data. The production-related sources were then grown to 2028 based on growth factors derived from the Annual Energy Outlook (AEO) 2018 data for oil, natural gas, or a combination thereof. The grown emissions were then controlled to account for the impacts of relevant New Source Performance Standards (NSPS).

Platform Sector: *abbreviation*	Description of Projection Method for regional haze case
Remaining non-EGU point: ***Ptnonipm***	First, known closures were applied to the 2016 ptnonipm sources. Closures were obtained from the Emission Inventory System (EIS) and also submitted by the states of Alabama, North Carolina, and Ohio. Industrial sources were grown using factors derived from the AEO 2018. Airport emissions were grown using factors derived from the Terminal Area Forecast (TAF) (see https://www.faa.gov/data_research/aviation/taf/). Rail yard emissions were grown using the same factors as line haul locomotives in the rail sector. Controls were then applied to account for relevant NSPS for reciprocating internal combustion engines (RICE), gas turbines, and process heaters. Reductions due to consent decrees that had not been fully implemented by 2016 were also applied, along with specific comments received by S/L/Ts.
Agricultural: ***Ag***	Livestock were projected based on factors created from USDA National livestock inventory projections published in February 2018 (https://www.ers.usda.gov/webdocs/publications/87459/oce-2018-1.pdf?v=0). Fertilizer emissions were held constant at year 2016 levels.
Area fugitive dust: ***Afdust***	Paved road dust was grown to 2028 levels based on the growth in VMT from 2016 to 2028. The remainder of the sector including building construction, road construction, agricultural dust, and road dust was held constant. The projected emissions are reduced during modeling according to a transport fraction (newly computed for the beta platform) and a meteorology-based (precipitation and snow/ice cover) zero-out as they are for the base year.
Category 1, 2 CMV: ***cmv_c1c2***	Category 1 (C1) and category 2 (C2) CMV emissions sources outside of California were projected to 2028 based on factors from the Regulatory Impact Analysis (RIA) Control of Emissions of Air Pollution from Locomotive Engines and Marine Compression Ignition Engines Less than 30 Liters per Cylinder. California emissions were projected based on factors provided by the state.
Category 3 CMV: ***cmv_c3***	Category 3 (C3) CMV emissions were projected using a forthcoming EPA report on projected bunker fuel demand. The report projects bunker fuel consumption by region out to the year 2030. Bunker fuel usage was used as a surrogate for marine vessel activity. Factors based on the report were used for all pollutants except NOx. Growth factors for NOx emissions were handled separately to account for the phase in of Tier 3 vessel engines. The NOx growth rates from the EPA C3 Regulatory Impact Assessment (RIA) were refactored to use the new bunker fuel usage growth rates. The assumptions of changes in fleet composition and emissions rates from the C3 RIA were preserved and applied to the new bunker fuel demand growth rates for 2028 to arrive at the final growth rates.
Locomotives: ***rail***	Passenger and freight were projected using separate factors with each factor applied to all pollutants. The factors are based on AEO2018, except the 2016-to-2017 trend for freight was based on historical fuel use for those years instead of AEO2018. In other words, the freight projection factors are based on 2016-to-2017 fuel use growth plus AEO2018 projections for 2017-to-future. Passenger train emissions were grown to 2028 by 16% and freight trains by 4.7%.
Remaining nonpoint: ***nonpt***	Industrial emissions were grown according to factors derived from AEO 2018. Portions of the nonpt sector were grown using factors based on expected growth in human population. Controls were applied to reflect relevant NSPS rules (i.e., reciprocating internal combustion engines (RICE), natural gas turbines, and process heaters). Emissions were also reduced to account fuel sulfur rules in the mid-Atlantic and northeast.

Platform Sector: *abbreviation*	**Description of Projection Method for regional haze case**
Nonpoint source oil and gas: *np_oilgas*	Production-related sources grown starting with an average of 2014 and 2016 production data. Emissions were initially projected to 2017 using historical data and then grown to 2028 based on factors generated based on AEO2018. Based on the SCC, factors related to oil, gas, or combined growth were used. Coalbed methane SCCs were projected independently. Controls were then applied to account for NSPS for oil and gas and RICE.
Residential Wood Combustion: *rwc*	RWC emissions were projected from 2014 to 2028 based on growth and control assumptions compatible with EPA's 2011v6.3 platform, which accounts for growth, retirements, and NSPS, although implemented in the Mid-Atlantic Regional Air Management Association (MARAMA)'s growth tool. RWC emissions in California, Oregon, and Washington were held constant.
Nonroad: *nonroad*	Outside California, the MOVES2014b model was run to create nonroad emissions for 2028 without any state inputs. The fuels used are specific to the future year, but the meteorological data represented the year 2016. For California, datasets provided by the California Air Resources Board (CARB) circa 2017 were used.
Onroad: *onroad*	Activity data were projected from 2016 to 2028 based on factors derived from AEO 2018. Where S/Ls provided activity data, those data were used. To create the emission factors, MOVES2014a was run for the year 2028, with 2016 met. data and fuels, but with the remaining inputs consistent with those used in 2014NEIv2. The future year activity data and emission factors were then combined using SMOKE-MOVES to produce the 2028 emissions.
Onroad California: *onroad_ca_adj*	CARB-provided emissions were used for California, but they were gridded and temporalized using MOVES2014a-based data output from SMOKE-MOVES. Volatile organic compound (VOC) HAP emissions derived from California-provided VOC emissions and MOVES-based speciation.
Other Area Fugitive dust sources not from the NEI: *othafdust*	Othafdust emissions for future years were provided by ECCC. The emissions were extracted from a broader nonpoint source inventory. Adjustments to construction dust were made to make those more consistent with the 2016 and ECCC 2010 inventories. Mexico emissions are not included in this sector.
Other Point Fugitive dust sources not from the NEI: *othptdust*	Wind erosion emissions were removed from the point fugitive dust inventory prior to regional haze modeling. Base year 2015 inventories with the rotated grid pattern removed were projected to 2028 based on factors provided by ECCC. A transport fraction adjustment is applied to the projected inventories along with a meteorology-based (precipitation and snow/ice cover) zero-out.
Other point sources not from the NEI: *othpt*	For agricultural sources that were originally developed on the rotated 10-km grid, the reallocated base year emissions were projected to 2028 using projection factors based on data provided by ECCC and applied by province, pollutant, and ECCC sub-class code. Airports were also projected from 2016 using ECCC-based factors. For the remaining sources in this sector, ECCC provided future year inventories. For Mexico sources, inventories projected from Mexico's 2008 inventory to 2025 and 2030 were interpolated to the year 2028. The Mexico 2014 CMV inventory was used as-is without any projections.
Other non-NEI nonpoint and nonroad: *othar*	Future year nonpoint inventories for many parts of this sector were provided by ECCC and were split into sectors to match those in the base year inventory. For Canadian nonroad sources, factors were provided from which the future year inventories could be derived. For Mexico nonpoint and nonroad sources, inventories projected to 2025 and 2030 from their 2008 inventory were interpolated to 2028. Mexico CMV emissions were removed so as not to double-count emissions in the othpt sector.

Platform Sector: ***abbreviation***	**Description of Projection Method for regional haze case**
Other non-NEI onroad sources: ***onroad_can***	For Canadian mobile onroad sources, future year inventories were derived from the base year 2015 inventory and data provided by ECCC. Projection factors were applied by province, sub-class code, and pollutant.
Other non-NEI onroad sources: ***onroad_mex***	Monthly year 2028 Mexico (municipio resolution) onroad mobile inventory was developed based on a run of MOVES-Mexico for 2028.

3 Emissions Modeling

The CMAQ and CAMx air quality models require 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. Emissions modeling sometimes 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. For additional details that may not be covered in this section, see the specification sheets provided with the 2016 beta platform as many will contain additional sector-specific information.

3.1 Emissions modeling Overview

SMOKE version 4.6 was used to process the raw emissions inventories into emissions inputs for each modeling sector into a format compatible with CMAQ, which were then converted to CAMx. 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.

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 with the columns as follows.

The "Spatial" column shows the spatial approach used: "point" indicates that SMOKE maps the source from a point location (i.e., latitude and longitude) to a grid cell; "surrogates" indicates that some or all of the sources use spatial surrogates to allocate county emissions to grid cells; and "area-to-point" indicates that some of the sources use the SMOKE area-to-point feature to grid the emissions (further described in Section 3.4.2).

The "Speciation" column indicates that all sectors use the SMOKE speciation step, though biogenics speciation is done within the Tmpbeis3 program and not as a separate SMOKE step.

The "Inventory resolution" column shows the inventory temporal resolution from which SMOKE needs to calculate hourly emissions. Note that for some sectors (e.g., onroad, beis), there is no input inventory;

instead, activity data and emission factors are used in combination with meteorological data to compute hourly emissions.

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

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

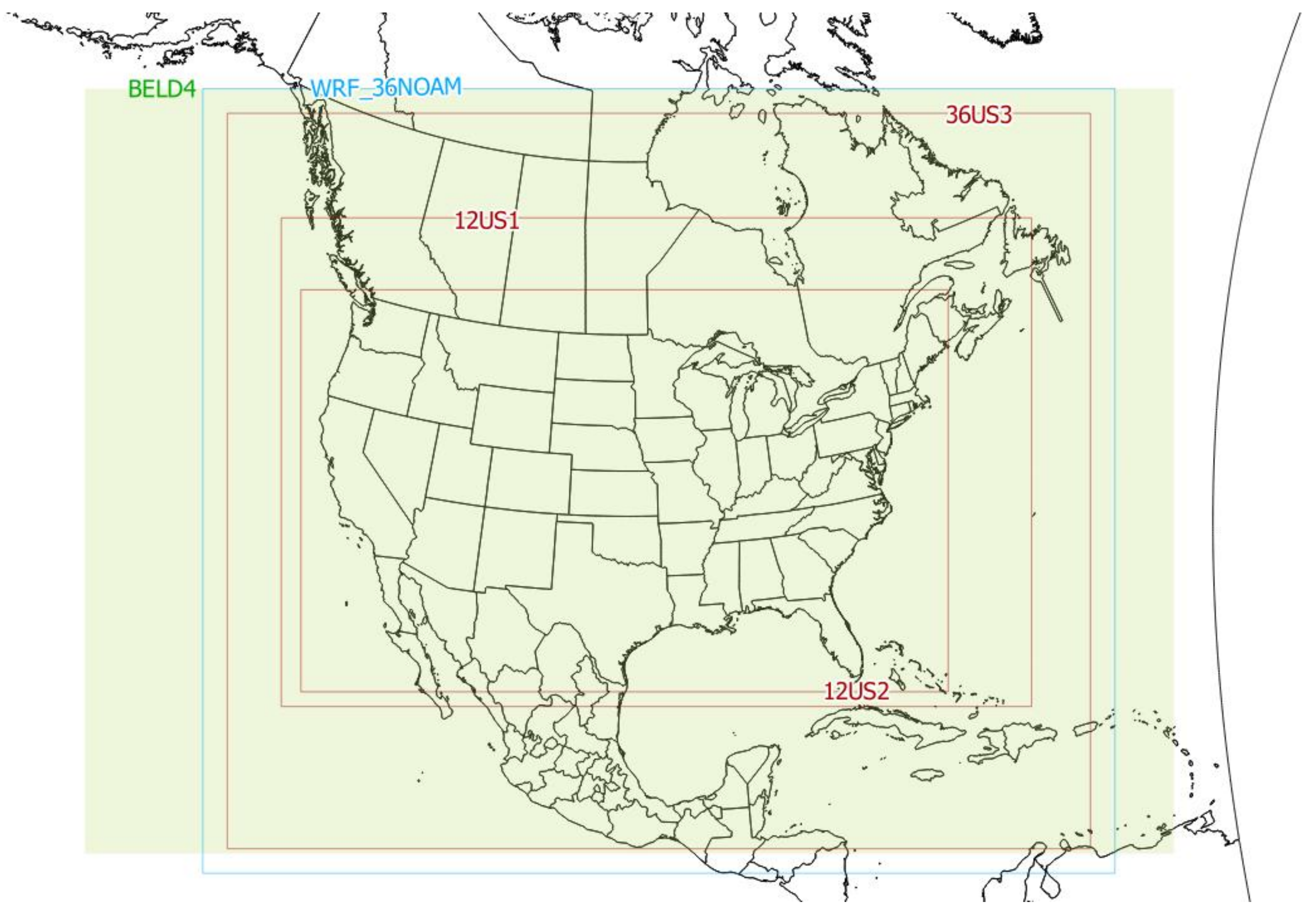
Platform sector	Spatial	Speciation	Inventory resolution	Plume rise
afdust_adj	Surrogates	Yes	annual	
ag	Surrogates	Yes	monthly	
beis	Pre-gridded land use	in BEIS3.61	computed hourly	
cmv_c1c2	Surrogates	Yes	annual	
cmv_c3	Point	Yes	annual	in-line
nonpt	Surrogates & area-to-point	Yes	annual	
nonroad	Surrogates & area-to-point	Yes	monthly	
np_oilgas	Surrogates	Yes	annual	
onroad	Surrogates	Yes	monthly activity, computed hourly	
onroad_ca_adj	Surrogates	Yes	monthly activity, computed hourly	
onroad_can	Surrogates	Yes	monthly	
onroad_mex	Surrogates	Yes	monthly	
othafdust_adj	Surrogates	Yes	annual	
othar	Surrogates	Yes	annual & monthly	
othpt	Point	Yes	annual & monthly	in-line
othptdust_adj	Point	Yes	monthly	None
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. When CAMx is the targeted air quality modeling, BEIS is run within SMOKE and the resulting emissions are included with the ground-level emissions input to CAMx.

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 two modeling domains: a 36-km resolution CONtinental United States "CONUS" modeling domain (36US3), and the 12-km resolution domain. 12US2. More specifically, SMOKE was run on the 12US1 domain and emissions were extracted from 12US1 data files to create 12US2 emission. The domains are shown in Figure 3-1.

Figure 3-1. Air quality modeling domains



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

Table 3-2. Descriptions of the platform grids

Common Name	Grid Cell Size	Description (see Figure 3-1)	Grid name	Parameters listed in SMOKE grid description (GRIDDESC) file: projection name, xorig, yorig, xcell, ycell, ncols, nrows, nthik
Continental 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 A.

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
	PTI	Titanium
Sea-salt species (non – anthropogenic) [4]	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 recent updates to speciation from previous platforms include the following:

- 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 and PM speciation process for nonroad mobile has been updated - profiles are now assigned within MOVES2014b 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;

[4] 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-speciated emissions; however for the 2015 inventory, 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 regional haze 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 integration[5]). For the "integrated" sources, SMOKE subtracts the "integrated" HAPs from the VOC (at the source level) to compute emissions for the new pollutant "NONHAPVOC." The user provides NONHAPVOC-to-NONHAPTOG factors and NONHAPTOG speciation profiles[6]. SMOKE computes NONHAPTOG and then applies the speciation profiles to allocate the NONHAPTOG to the other air quality model VOC

[5] 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.

[6] 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

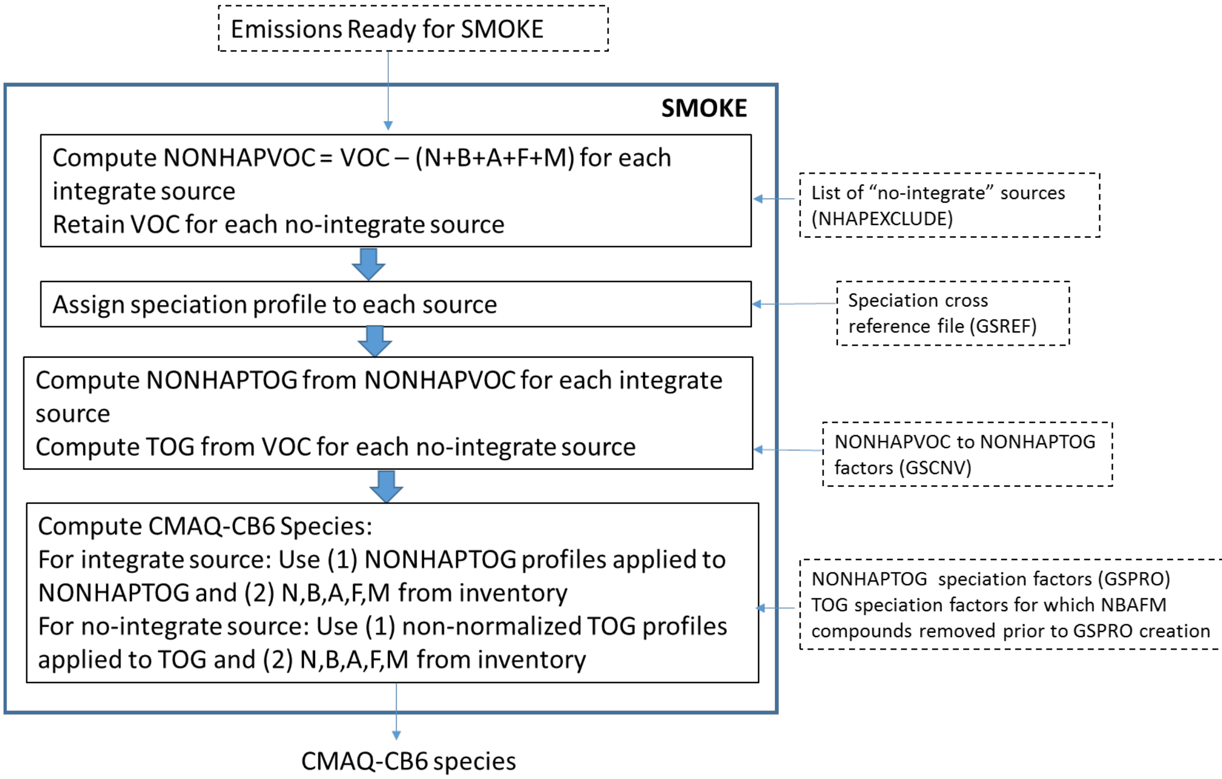


Table 3-4. Integration status of naphthalene, benzene, acetaldehyde, formaldehyde and methanol (NBAFM) for each platform sector

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
othptdust	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.

New in the 2016v7.2 beta and regional haze platforms, a GSPRO_COMBO is used to specify a mix of E0 and E10 fuels in Canada. ECCC provided percentages of ethanol use by province, and these were converted into E0 and E10 splits. For example, Alberta has 4.91% ethanol in its fuel, so we applied a mix of 49.1% E10 profiles (4.91% times 10, since 10% ethanol would mean 100% E10), and 50.9% E0 fuel. Ethanol splits for all provinces in Canada are listed in Table 3-5. The Canadian onroad inventory includes four distinct FIPS codes in Ontario, allowing for application of different E0/E10 splits in Southern Ontario versus Northern Ontario. In Mexico, only E0 profiles are used.

Table 3-5. Ethanol percentages by volume by Canadian province

Province	Ethanol % by volume (E10 = 10%)
Alberta	4.91%
British Columbia	5.57%
Manitoba	9.12%
New Brunswick	4.75%
Newfoundland & Labrador	0.00%
Nova Scotia	0.00%
NW Territories	0.00%
Nunavut	0.00%
Ontario (Northern)	0.00%
Ontario (Southern)	7.93%
Prince Edward Island	0.00%
Québec	3.36%
Saskatchewan	7.73%
Yukon	0.00%

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 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)[7]. SMOKE essentially calculates the model-ready species by using the appropriate emission factor without further speciation[8]. Third, MOVES' internal speciation uses full integration of an extended list of HAPs beyond NBAFM (called "M-profiles"). The M-profiles integration is very similar to NBAFM integration explained above except that the integration calculation (see Figure 3-2. Process of integrating NBAFM with VOC for use in VOC Speciation) is performed on emissions factors instead of on emissions, and a much larger set of pollutants are integrated besides NBAFM. The list of integrated pollutants is described in Table 3-6. 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. 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 3-6. 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

[7] 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.
[8] 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/.

MOVES ID	Pollutant Name
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 3-6. 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 3-6 was used. However, MOVES-MEXICO used CB6-CAMx, not CB6-CMAQ, so post-SMOKE we converted the emissions to CB6-CMAQ as follows:

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

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

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

For the biog sector, the speciation profiles used by BEIS are not included in SPECIATE. 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 recently added VOC profiles from SPECIATE4.5 (listed in Appendix B) are in 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 3-7 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. Oil and gas SCCs for associated gas, condensate tanks, crude oil tanks, dehydrators, liquids unloading and well completions represent the total VOC from the process, including the portions of process that may be flared or directed to a reboiler. For example, SCC 2310021400 (gas well dehydrators) consists of process, reboiler, and/or flaring emissions. There are not separate SCCs for the flared portion of the process or the reboiler. However, the VOC associated with these three portions can have very different speciation profiles. Therefore, it is necessary to have an estimate of the amount of VOC from each of the portions (process, flare, reboiler) so that the appropriate speciation profiles can be applied to each portion. The Nonpoint Oil and Gas Emission Estimation Tool generates an intermediate file which file provides flare, non-flare (process), and reboiler (for dehydrators) emissions for six source categories that have flare emissions: by county FIPS and SCC code for the U.S. From these emissions we can compute the fraction of the emissions to assign to each profile. These fractions can vary by county FIPS, because they depend on the level of controls which is an input to the Speciation Tool.

Table 3-7. Basin/Region-specific profiles for oil and gas

Profile Code	Description	Region (if not in the profile name)
DJVNT_R	Denver-Julesburg Basin Produced Gas Composition from Non-CBM Gas Wells	
PNC01_R	Piceance Basin Produced Gas Composition from Non-CBM Gas Wells	
PNC02_R	Piceance Basin Produced Gas Composition from Oil Wells	
PNC03_R	Piceance Basin Flash Gas Composition for Condensate Tank	
PNCDH	Piceance Basin, Glycol Dehydrator	
PRBCB_R	Powder River Basin Produced Gas Composition from CBM Wells	
PRBCO_R	Powder River Basin Produced Gas Composition from Non-CBM Wells	
PRM01_R	Permian Basin Produced Gas Composition for Non-CBM Wells	
SSJCB_R	South San Juan Basin Produced Gas Composition from CBM Wells	
SSJCO_R	South San Juan Basin Produced Gas Composition from Non-CBM Gas Wells	
SWFLA_R	SW Wyoming Basin Flash Gas Composition for Condensate Tanks	
SWVNT_R	SW Wyoming Basin Produced Gas Composition from Non-CBM Wells	

Profile Code	Description	Region (if not in the profile name)
UNT01_R	Uinta Basin Produced Gas Composition from CBM Wells	
WRBCO_R	Wind River Basin Produced Gagres Composition from Non-CBM Gas Wells	
95087a	Oil and Gas - Composite - Oil Field - Oil Tank Battery Vent Gas	East Texas
95109a	Oil and Gas - Composite - Oil Field - Condensate Tank Battery Vent Gas	East Texas
95417	Uinta Basin, Untreated Natural Gas	
95418	Uinta Basin, Condensate Tank Natural Gas	
95419	Uinta Basin, Oil Tank Natural Gas	
95420	Uinta Basin, Glycol Dehydrator	
95398	Composite Profile - Oil and Natural Gas Production - Condensate Tanks	Denver-Julesburg Basin
95399	Composite Profile - Oil Field – Wells	State of California
95400	Composite Profile - Oil Field – Tanks	State of California
95403	Composite Profile - Gas Wells	San Joaquin Basin

3.2.1.4 Mobile source related VOC speciation profiles

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

The VOC speciation profiles for the nonroad sector other than for California are listed in Table 3-8. 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 3-9.

Table 3-8. 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

Profile	Profile Description	Engine Type	Engine Technology	Engine Size	Horse-power category	Fuel	Fuel Sub-type	Emission Process
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 C.

Table 3-9 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 3-9. Select mobile-related VOC profiles 2016

Sector	Sub-category	2014	
Nonroad- California & non US	gasoline exhaust	COMBO	
		8750a	Pre-Tier 2 E0 exhaust
		8751a	Pre-Tier 2 E10 exhaust
Nonroad-California	gasoline evaporative	COMBO	
		8753	E0 evap
		8754	E10 evap
Nonroad-California	gasoline refueling	COMBO	
		8869	E0 Headspace
		8870	E10 Headspace
Nonroad-California	diesel exhaust	8774	Pre-2007 MY HDD exhaust
Nonroad-California	diesel evap-orative and diesel refueling	4547	Diesel Headspace
	PFC and BTP	COMBO	

Sector	Sub-category	2014	
nonpt/ ptnonipm		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 3-10 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 3-11 through Table 3-13 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 3-10. Onroad M-profiles

Profile	Profile Description	Model Years	ProcessID	FuelSubTypeID	RegClassID
1001M	CNG Exhaust	1940-2050	1,2,15,16	30	48
4547M	Diesel Headspace	1940-2050	11	20,21,22	0
4547M	Diesel Headspace	1940-2050	12,13,18,19	20,21,22	10,20,30,40,41, 42,46,47,48
8753M	E0 Evap	1940-2050	12,13,19	10	10,20,30,40,41,42, 46,47,48
8754M	E10 Evap	1940-2050	12,13,19	12,13,14	10,20,30,40,41, 42,46,47,48
8756M	Tier 2 E0 Exhaust	2001-2050	1,2,15,16	10	20,30
8757M	Tier 2 E10 Exhaust	2001-2050	1,2,15,16	12,13,14	20,30
8758M	Tier 2 E15 Exhaust	1940-2050	1,2,15,16	15,18	10,20,30,40,41, 42,46,47,48
8766M	E0 evap permeation	1940-2050	11	10	0
8769M	E10 evap permeation	1940-2050	11	12,13,14	0
8770M	E15 evap permeation	1940-2050	11	15,18	0
8774M	Pre-2007 MY HDD exhaust	1940-2006	1,2,15,16,17,90	20, 21, 22	40,41,42,46,47, 48
8774M	Pre-2007 MY HDD exhaust	1940-2050	91[9]	20, 21, 22	46,47
8774M	Pre-2007 MY HDD exhaust	1940-2006	1,2,15,16	20, 21, 22	20,30

[9] 91 is the processed for APUs which are diesel engines not covered by the 2007 Heavy-Duty Rule, so the older technology applieds to all years.

Profile	Profile Description	Model Years	ProcessID	FuelSubTypeID	RegClassID
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[10]	10,40,41,42,46,47,48

Table 3-11. MOVES process IDs

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

[10] The profile assingments 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.

40	Nonroad
90	Extended Idle Exhaust
91	Auxiliary Power Exhaust

Table 3-12. 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 3-13. 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)

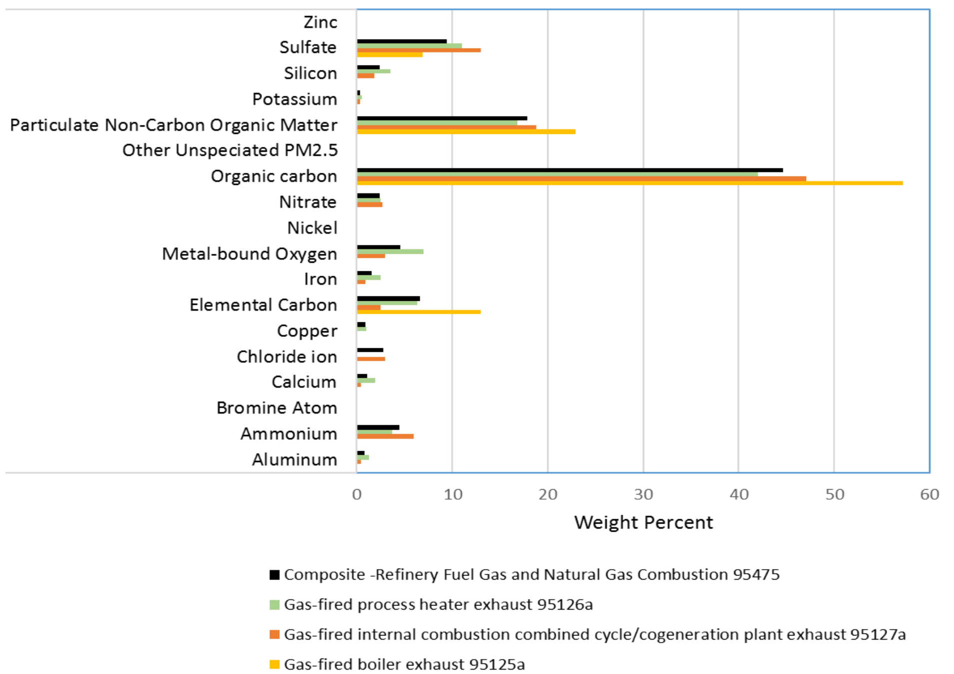
For portable fuel containers (PFCs) and fuel distribution operations associated with the bulk-plant-to-pump (BTP) distribution, ethanol may be mixed into the fuels; therefore, county- and month-specific COMBO speciation was used (via the GSPRO_COMBO file). Refinery to bulk terminal (RBT) fuel distribution 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 $PM_{2.5}$. $PM_{2.5}$ was speciated into the AE6 species associated with CMAQ 5.0.1 and later versions. Of particular note for the 2016v7.2 beta and regional haze platforms, the nonroad $PM_{2.5}$ speciation was updated as discussed later in this section. Most of the PM profiles come from the 911XX series (Reff et. al, 2009), which include updated AE6 speciation[11]. 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.

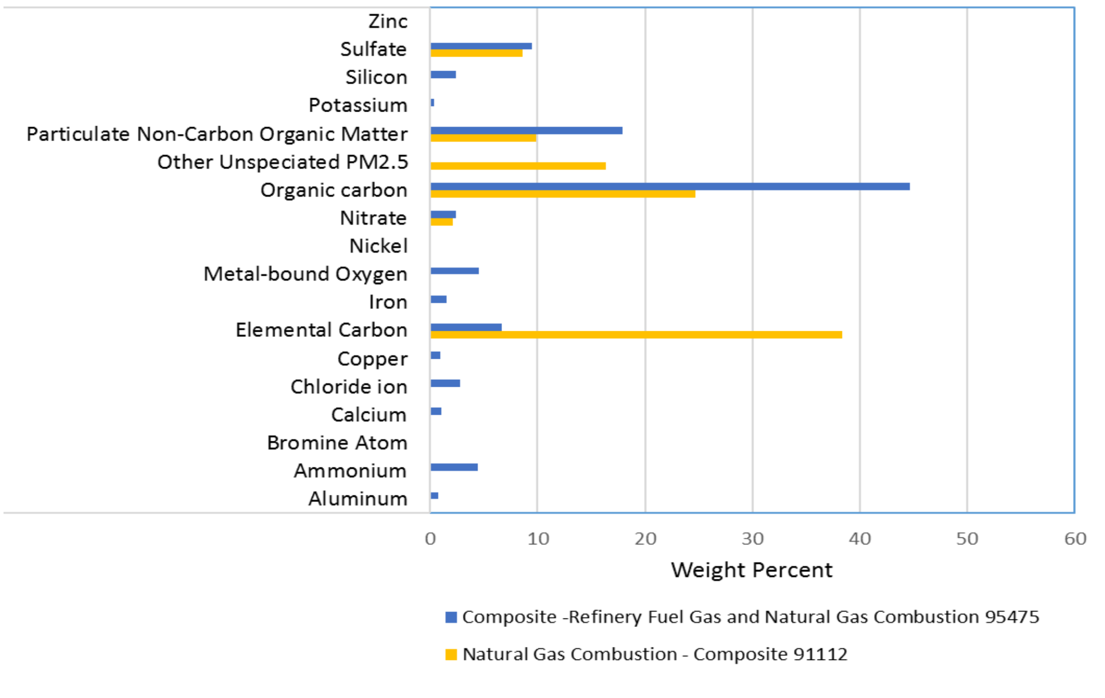
Profile 95475 (Composite -Refinery Fuel Gas and Natural Gas Combustion) is shown along with the underlying profiles composited in Figure 3-3. Figure 3-4 shows a comparison of the new profile as of the 2014v7.1 platform with the one that we had been using in the 2014v7.0 and earlier platforms.

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



[11] 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 3-4. Comparison of PM profiles used for Natural gas combustion related sources



3.2.2.1 Mobile source related PM2.5 speciation profiles

For the onroad sector, for all processes except brake and tire wear, PM speciation occurs within MOVES itself, not within SMOKE (similar to the VOC speciation described above). The advantage of using MOVES to speciate PM is that during the internal calculation of MOVES, the model has complete information on the characteristics of the fleet and fuels (e.g., model year, sulfur content, process, etc.) to accurately match to specific profiles. This means that MOVES produces EF tables that include total PM (e.g., PM_{10} and $PM_{2.5}$) and speciated PM (e.g., PEC, PFE, etc). SMOKE essentially calculates the PM components by using the appropriate EF without further speciation[12]. 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 3-14 shows the differences in the v7.1 and v6.3 profiles.

[12] 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/.

Table 3-14. SPECIATE4.5 brake and tire profiles compared to those used in the 2011v6.3 Platform

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

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

```
POC = 0.6395 * PM25TIRE + 0.0503 * PM25BRAKE
PEC = 0.0036 * PM25TIRE + 0.0128 * PM25BRAKE
PNO3 = 0.000 * PM25TIRE + 0.000 * PM25BRAKE
PSO4 = 0.0 * PM25TIRE + 0.0 * PM25BRAKE
PNH4 = 0.000 * PM25TIRE + 0.0000 * PM25BRAKE
PNCOM = 0.2558 * PM25TIRE + 0.0201 * PM25BRAKE
```

For California onroad emissions, adjustment factors were applied to SMOKE-MOVES to produce California adjusted model-ready files. 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 partially done within MOVES such that it does not need to be run for a specific chemical mechanism. For nonroad, MOVES outputs emissions of PM2.5 split by speciation profile. Similar to how VOC and NONHAPTOG are speciated, PM2.5 is now also speciated this way starting with MOVES2014b. California nonroad emissions, which are not from MOVES, continue to be speciated the traditional way with speciation profiles assigned by SMOKE using the GSREF cross-reference. The PM2.5 profiles assigned to nonroad sources are listed in Table 3-15.

Table 3-15. Nonroad PM2.5 profiles

SPECIATE4.5 Profile Code	SPECIATE4.5 Profile Name	Assigned to Nonroad sources based on Fuel Type
8996	Diesel Exhaust - Heavy-heavy duty truck - 2007 model year with NCOM	Diesel
91106	HDDV Exhaust – Composite	Diesel
91113	Nonroad Gasoline Exhaust – Composite	Gasoline
91156	Residential Natural Gas Combustion	CNG and LPG (California only)
95219	CNG Transit Bus Exhaust	CNG and LPG

3.2.3 NO_X speciation

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

The importance of HONO chemistry, identification of its presence in ambient air and the measurements of HONO from mobile sources have prompted the inclusion of HONO in NOx speciation for mobile sources. Based on tunnel studies, a HONO to NOx ratio of 0.008 was chosen (Sarwar, 2008). For the mobile sources, except for onroad (including nonroad, cmv, rail, othon sectors), and for specific SCCs in othar and ptnonipm, the profile "HONO" is used. Table 3-16 gives the split factor for these two profiles. The onroad sector does not use the "HONO" profile to speciate NO_X. MOVES2014 produces speciated NO, NO_2, and HONO by source, including emission factors for these species in the emission factor tables used by SMOKE-MOVES. Within MOVES, the HONO fraction is a constant 0.008 of NO_X. The NO fraction varies by heavy duty versus light duty, fuel type, and model year.
The NO_2 fraction = 1 – NO – HONO. For more details on the NO_X fractions within MOVES, see https://nepis.epa.gov/Exe/ZyPDF.cgi?Dockey=P100F1A5.pdf .

Table 3-16. NO_X speciation profiles

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

3.2.4 Creation of Sulfuric Acid Vapor (SULF)

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

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

$$
\begin{aligned}
&\mathit{Emissions\ of\ SULF}\ (\mathit{as}\ \mathrm{H2SO4}) \\
&\qquad = \mathit{SO2\ emissions} \times \frac{\mathit{fraction\ of\ S\ emitted\ as\ sulfate}}{\mathit{fraction\ of\ S\ emitted\ as\ SO2}} \times \frac{\mathit{MW\ H2SO4}}{\mathit{MW\ SO2}}
\end{aligned}
$$

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

This method does not reduce SO_2 emissions; it solely adds gaseous sulfate emissions as a function of SO2 emissions. The derivation of the profiles is provided in Table 3-17; a summary of the profiles is provided in Table 3-18.

Table 3-17. Sulfate split factor computation

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

Table 3-18. SO_2 speciation profiles

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

3.3 Temporal Allocation

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

The temporal factors applied to the inventory are selected using some combination of country, state, county, SCC, and pollutant. Table 3-19 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 3-19. 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_c1c2	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
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
othptdust_adj	Monthly	No	week	all	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

Platform sector short name	Inventory resolutions	Monthly profiles used?	Daily temporal approach	Merge processing approach	Process holidays as separate days
ptfire_othna	Daily	No	all	all	No
rail	Annual	Yes	aveday	aveday	No
rwc	Annual	No[3]	met-based[3]	all	No[3]

[1]Note the annual and monthly "inventory" actually refers to the activity data (VMT, hoteling and VPOP) for onroad. VMT and hoteling is monthly and VPOP is annual. The actual emissions are computed on an hourly basis.
[2]Only units that do not have matching hourly CEMS data use monthly temporal profiles.
[3]Except for 2 SCCs that do not use met-based 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 SO_2 inventory data for the seasons in which the CEMS are operating. If a CEMS-matched unit is determined to be a partial year reporter, as can happen for sources that run CEMS only in the summer, emissions totaling the difference between the annual emissions and the total CEMS emissions are allocated to the non-summer months.

Figure 3-5. Eliminating unmeasured spikes in CEMS data

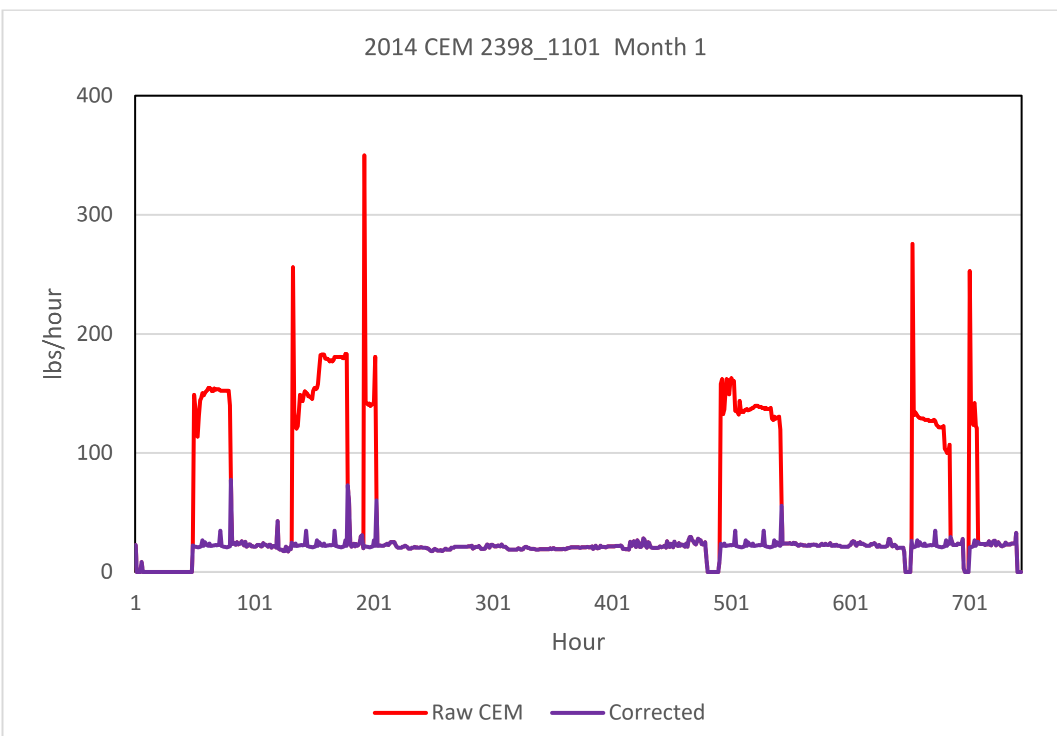
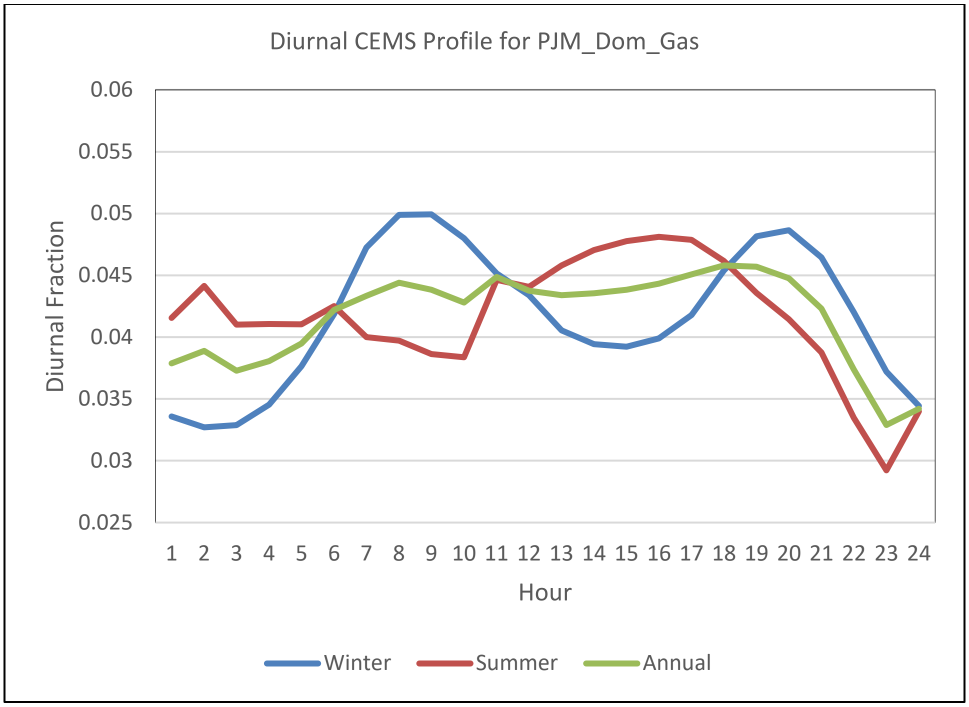


Figure 3-6. Seasonal diurnal profiles for EGU emissions in a Virginia Region



For sources not matched to CEMS units, temporal profiles are calculated that are used by SMOKE to allocate the annual emissions to hourly values. For these units, the allocation of the inventory annual emissions to months is done using average fuel-specific annual-to-month factors generated for regions with similar climate. 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, SO_2, and heat input. An overall composite profile was also computed and used when there were no CEMS units with the specified fuel in the region containing the unit. For both CEMS-matched units and units not matched to CEMS, NO_X and SO_2 CEMS data are used to allocate NO_X and SO_2 emissions to monthly emissions, respectively, while heat input data are used to allocate emissions of all pollutants from monthly to daily emissions.

Daily temporal allocation of units matched to CEMS was performed using a procedure similar to the approach to allocate emissions to months in that the CEMS data replaces the inventory data for each pollutant. For units without CEMS data, emissions were allocated from month to day using IPM-region and fuel-specific average month-to-day factors based on the 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 SO_2 CEMS data are used to replace inventory NO_X and SO_2 emissions, while CEMS heat input data are used to allocate all other pollutants.

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

For additional information on EGU temporal allocation, please see the Point-EGU-IPM specification sheet provided with the 2016 beta platform.

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 3-7 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 3-7, Figure 3-8, and Figure 3-9. 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 3-10. These were assigned based on the facility ID.

Figure 3-7. Diurnal Profile for all Airport SCCs

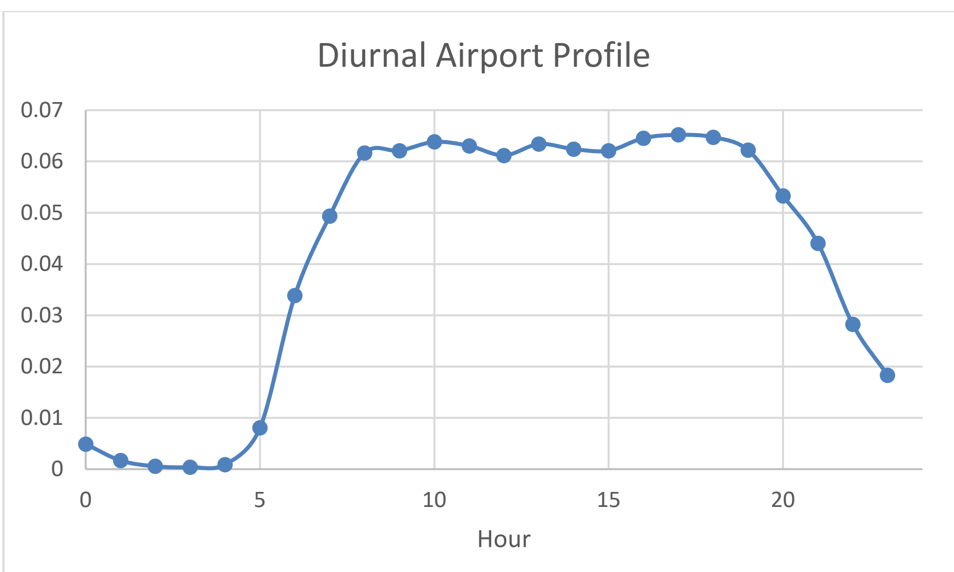


Figure 3-8. Weekly profile for all Airport SCCs

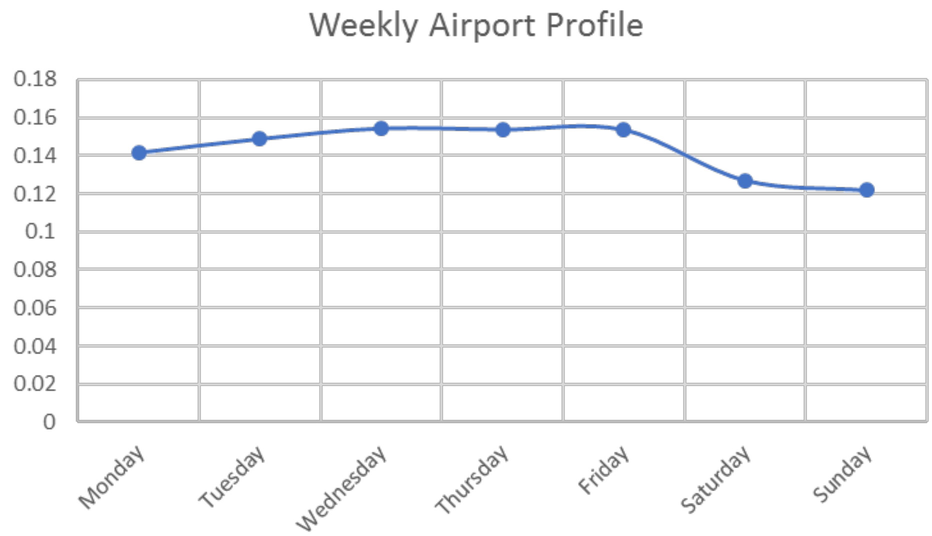


Figure 3-9. Monthly Profile for all Airport SCCs

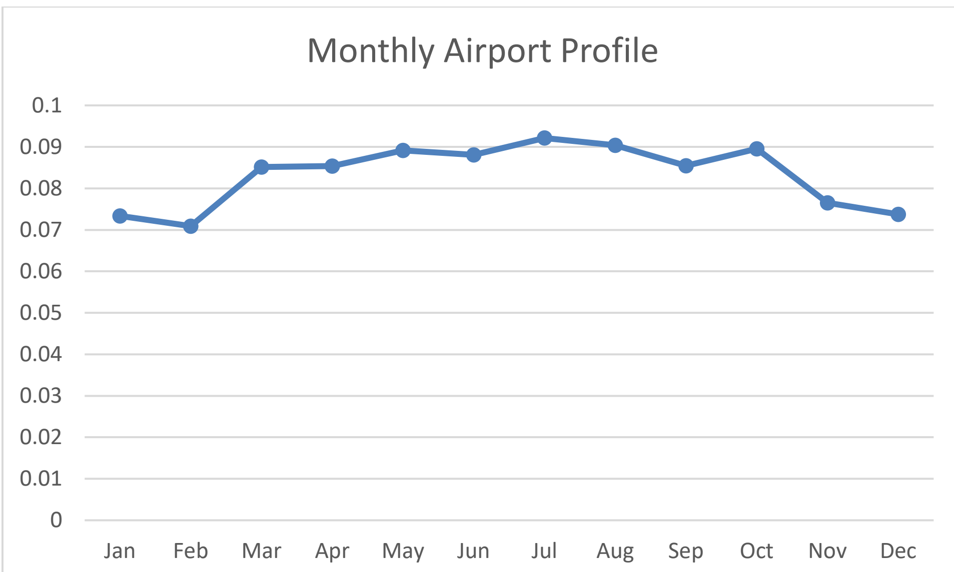
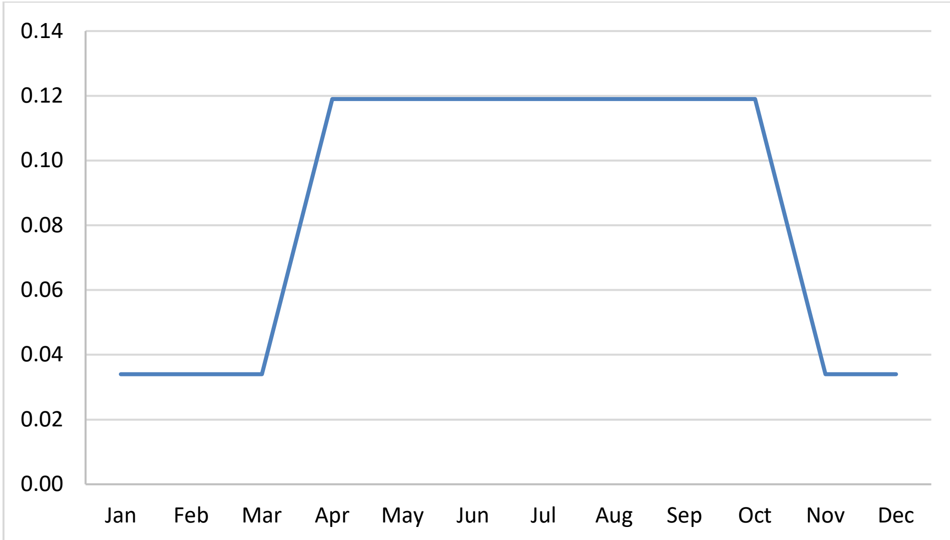


Figure 3-10. Alaska Seaplane Profile



3.3.4 Residential Wood Combustion Temporal allocation (rwc)

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

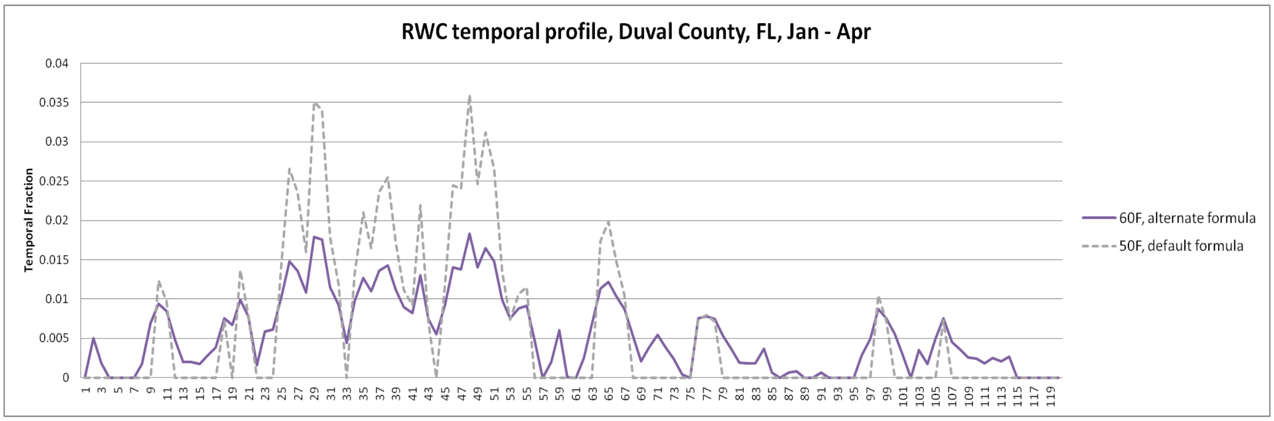
The SMOKE program Gentpro provides a method for developing meteorology-based temporal allocation. Currently, the program can utilize three types of temporal algorithms: annual-to-day temporal allocation for residential wood combustion (RWC); month-to-hour temporal allocation for agricultural livestock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

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

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

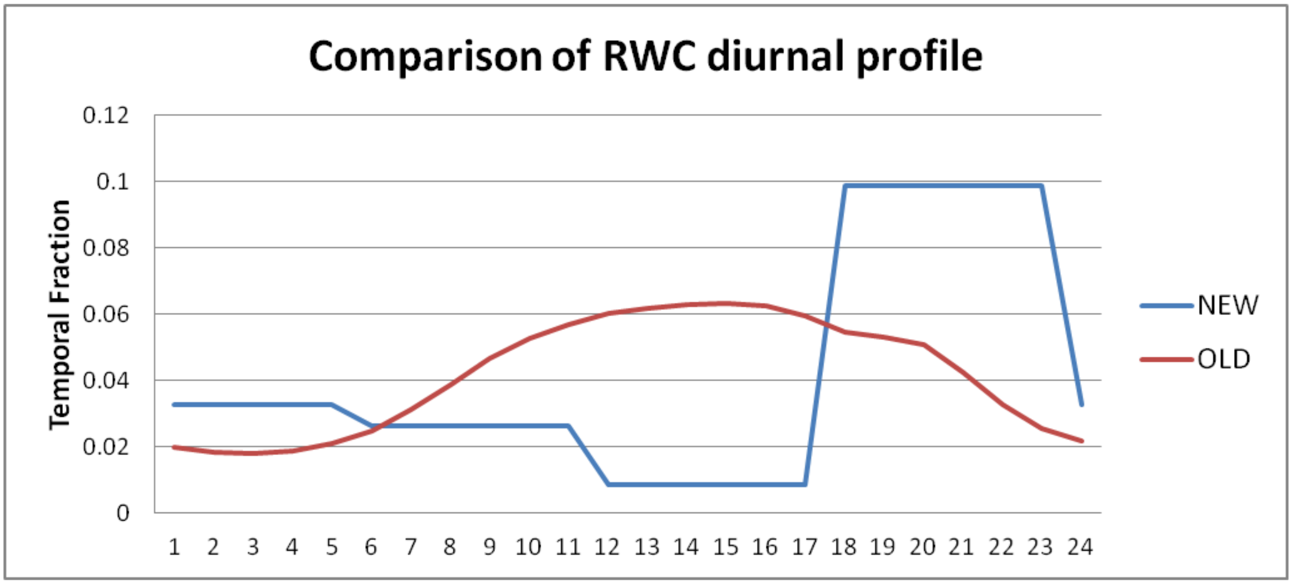
Figure 3-11 illustrates the impact of changing the temperature threshold for a warm climate county. The plot shows the temporal fraction by day for Duval County, Florida, for the first four months of 2007. The default 50 ˚F threshold creates large spikes on a few days, while the 60 ˚F threshold dampens these spikes and distributes a small amount of emissions to the days that have a minimum temperature between 50 and 60 ˚F.

Figure 3-11. 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 3-12) 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 3-12. 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 create the diurnal profile for OHH, shown in Figure 3-13, are based on a conventional single-stage heat load unit burning red oak in Syracuse, New York. As shown in Figure 3-14, 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 3-15. 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 3-13. Data used to produce a diurnal profile for OHH, based on heat load (BTU/hr)

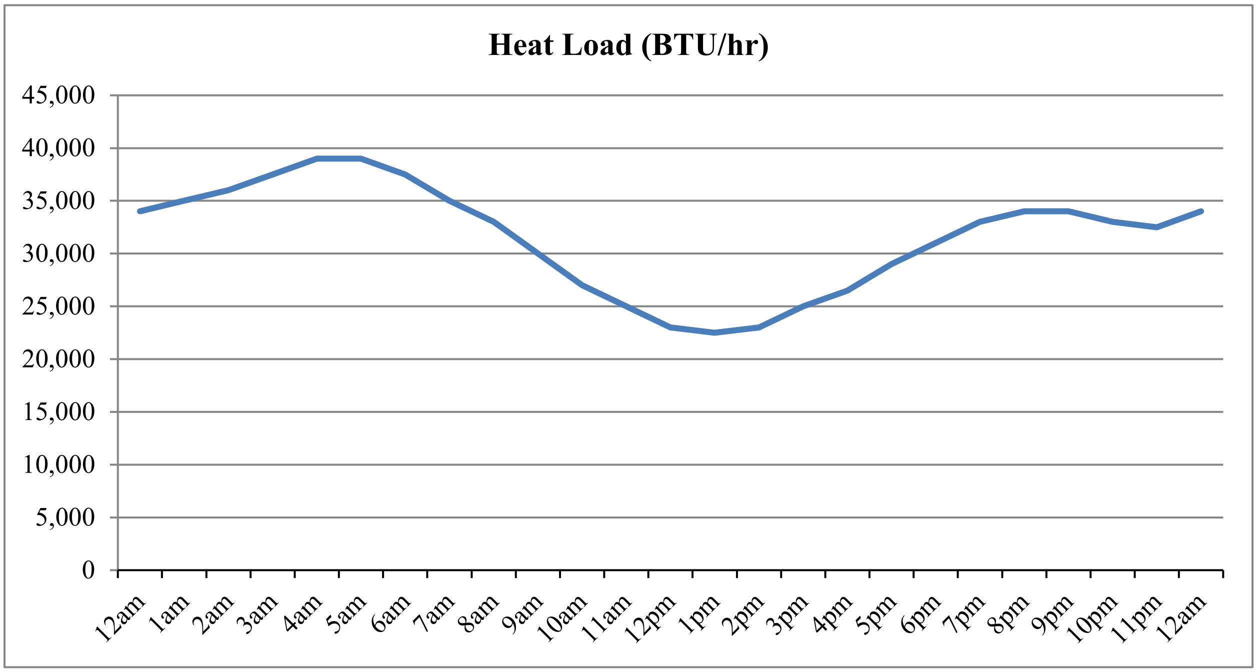


Figure 3-14. Day-of-week temporal profiles for OHH and Recreational RWC

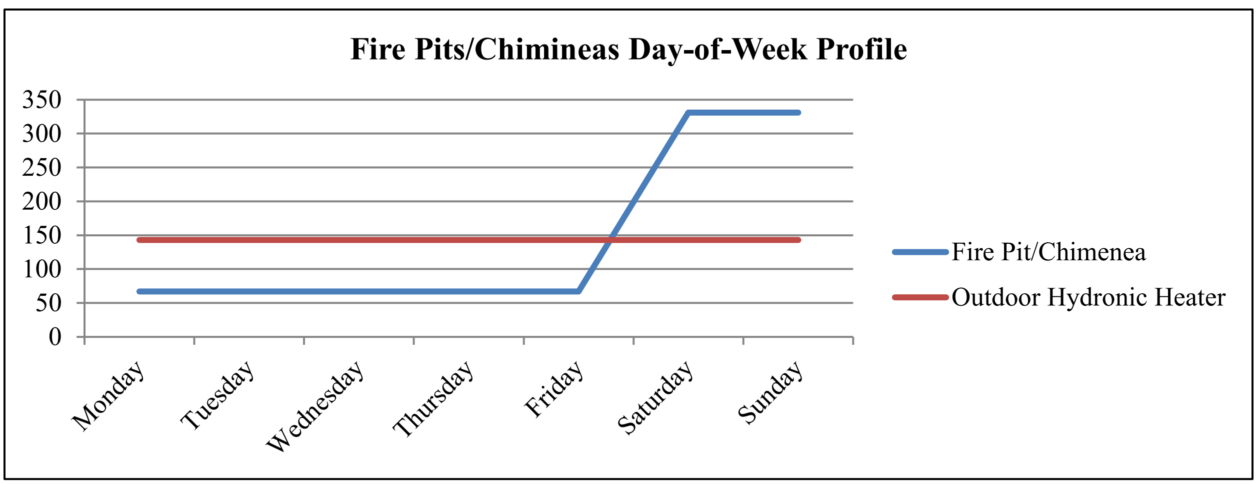
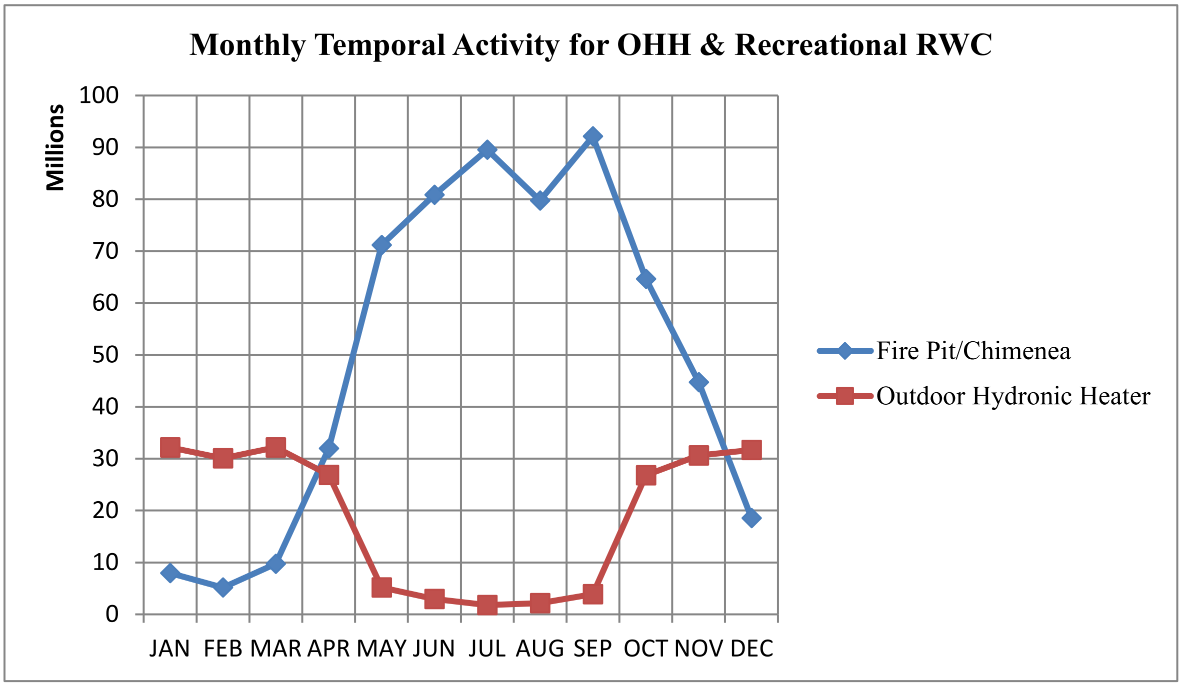


Figure 3-15. Annual-to-month temporal profiles for OHH and recreational RWC



3.3.5 Agricultural Ammonia Temporal Profiles (ag)

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

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

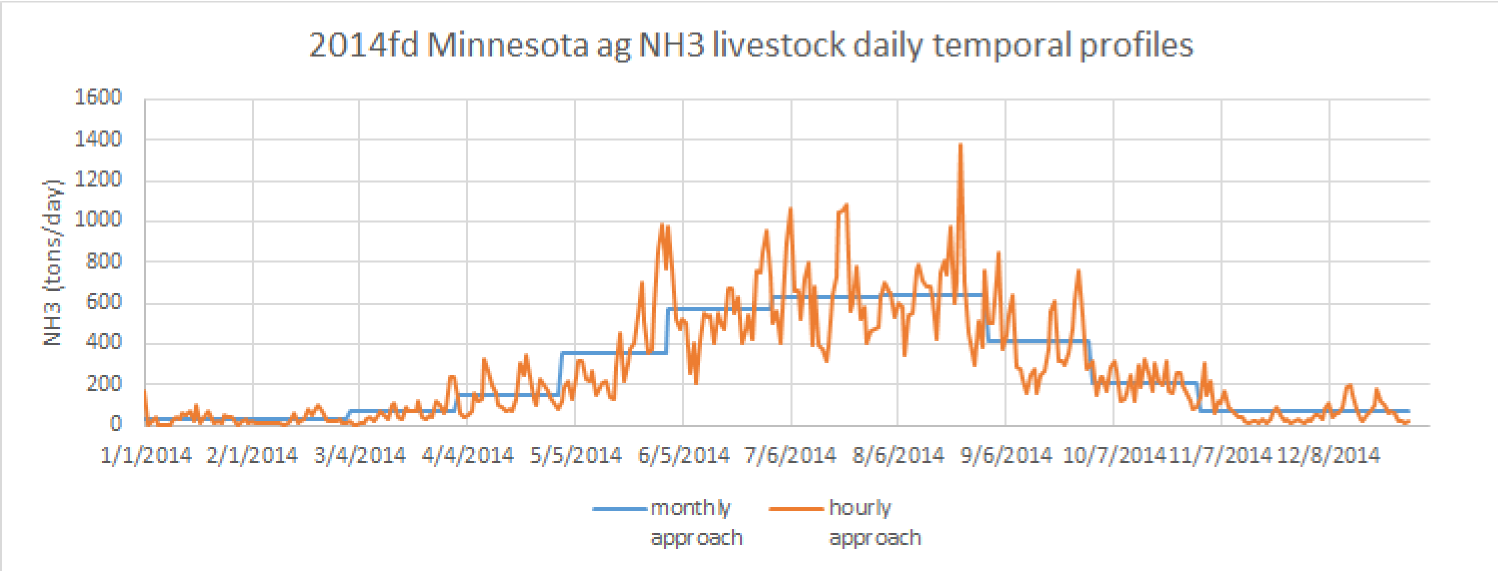
$$PE_{i,h} = E_{i,h} / \text{Sum}(E_{i,h})$$

where

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

GenTPRO was run using the "BASH_NH3" profile method to create month-to-hour temporal profiles for these sources. Because these profiles distribute to the hour based on monthly emissions, the monthly emissions are obtained from a monthly inventory, or from an annual inventory that has been temporalized to the month. Figure 3-16 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 3-16. Example of animal NH_3 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, NH_3 and non- NH_3, livestock and fertilizer. Monthly profiles are based on the daily-based EPA livestock emissions and are the same as were used in 2014v7.0. Profiles are by state/SCC_category, where SCC_category is one of the following: beef, broilers, layers, dairy, swine.

3.3.6 Oil and gas temporal allocation (np_oilgas)

Monthly oil and gas temporal profiles by county and SCC were updated to use 2016 activity information for the beta and regional haze cases. 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)

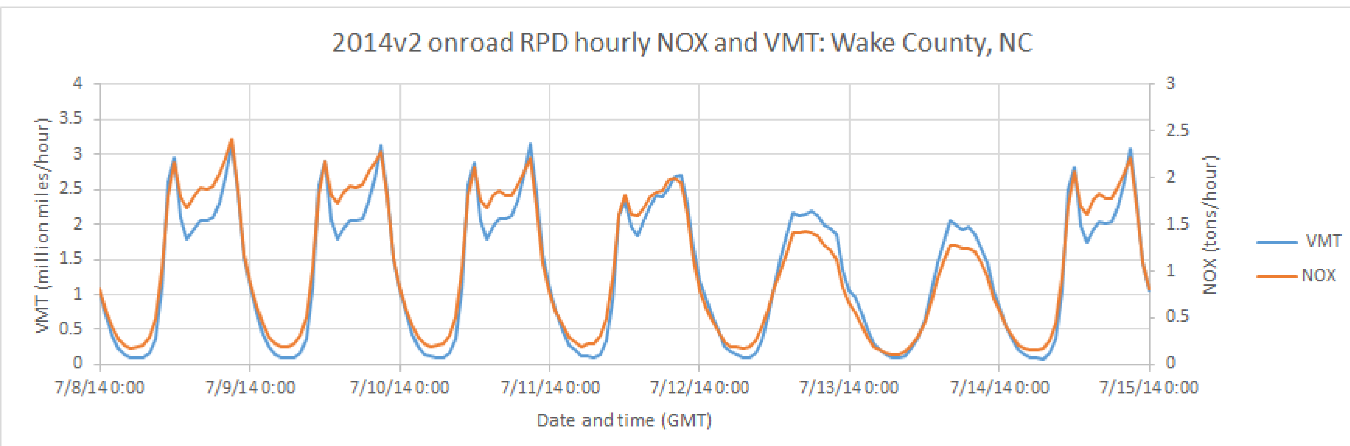
For the onroad sector, the temporal distribution of emissions is a combination of traditional temporal profiles and the influence of meteorology. This section will discuss both the meteorological influences and the development of the temporal profiles for this platform.

The “inventories” referred to in Table 3-19 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 3-17 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 3-17. Example of temporal variability of NOx 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 3-18. 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 3-19 shows which counties have temporal profiles specific to that county, and which counties use regional average profiles.

Figure 3-18. Sample onroad diurnal profiles for Fulton County, GA

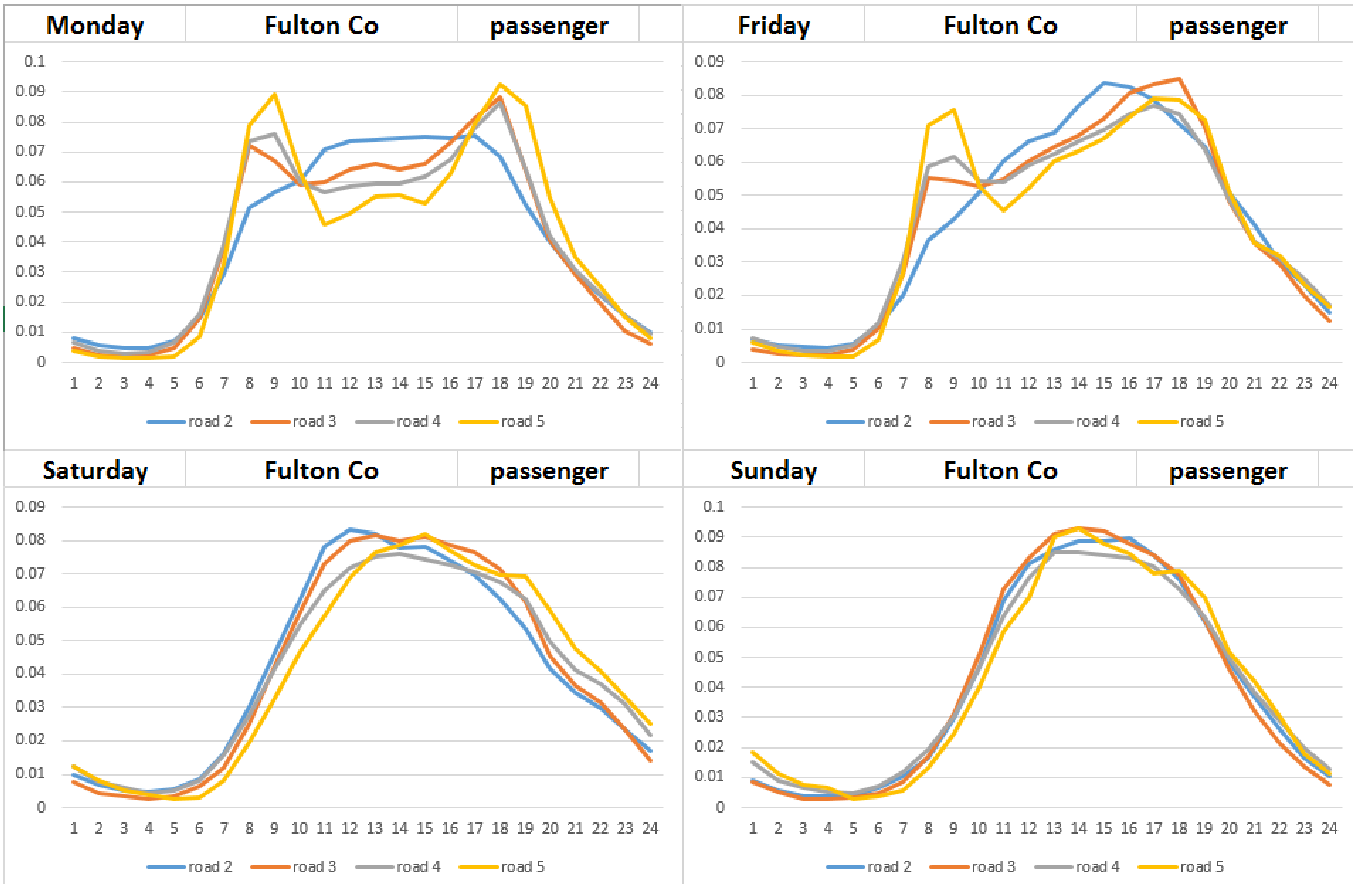
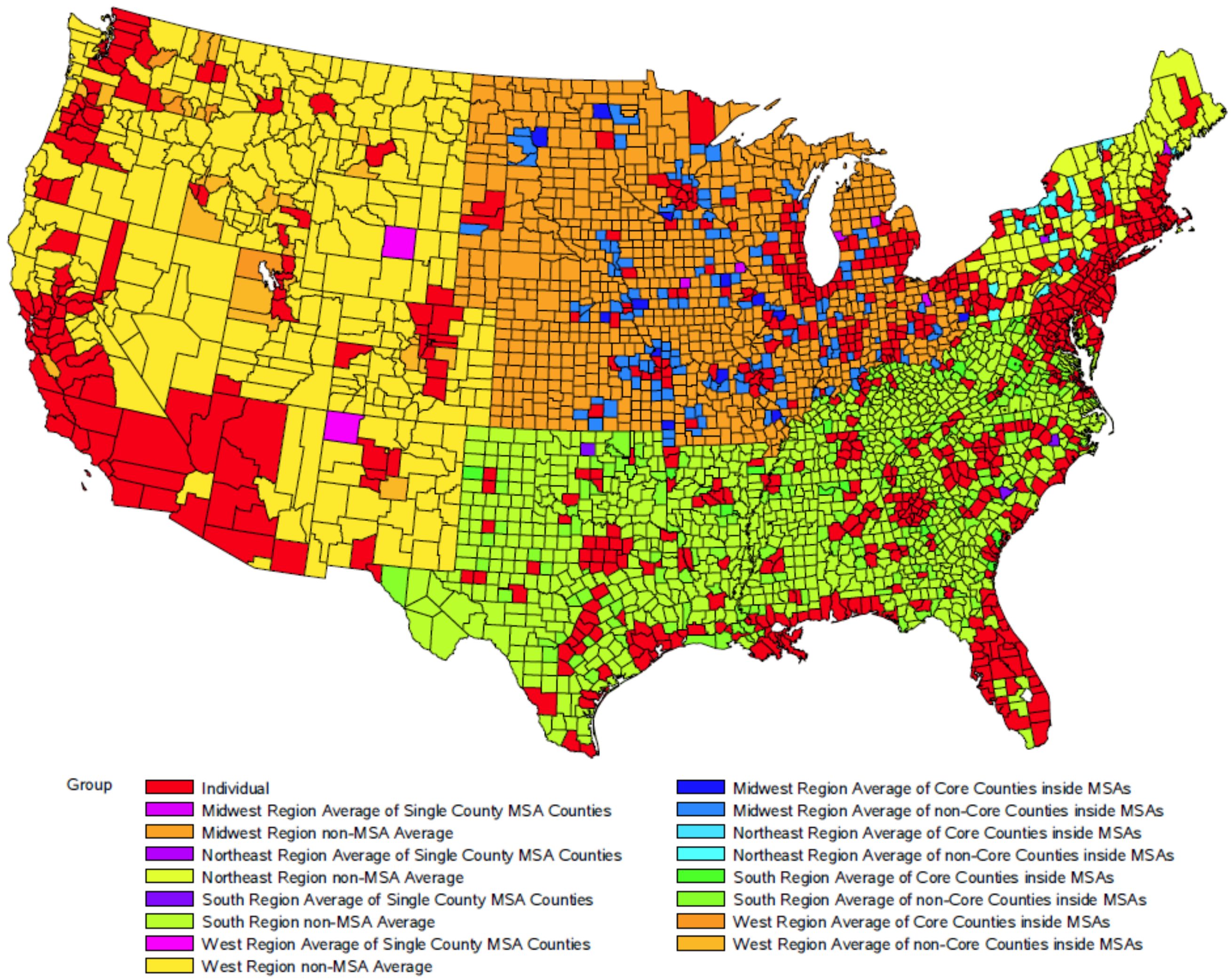


Figure 3-19. Counties for which MOVES Speeds and Temporal Profiles could be Populated

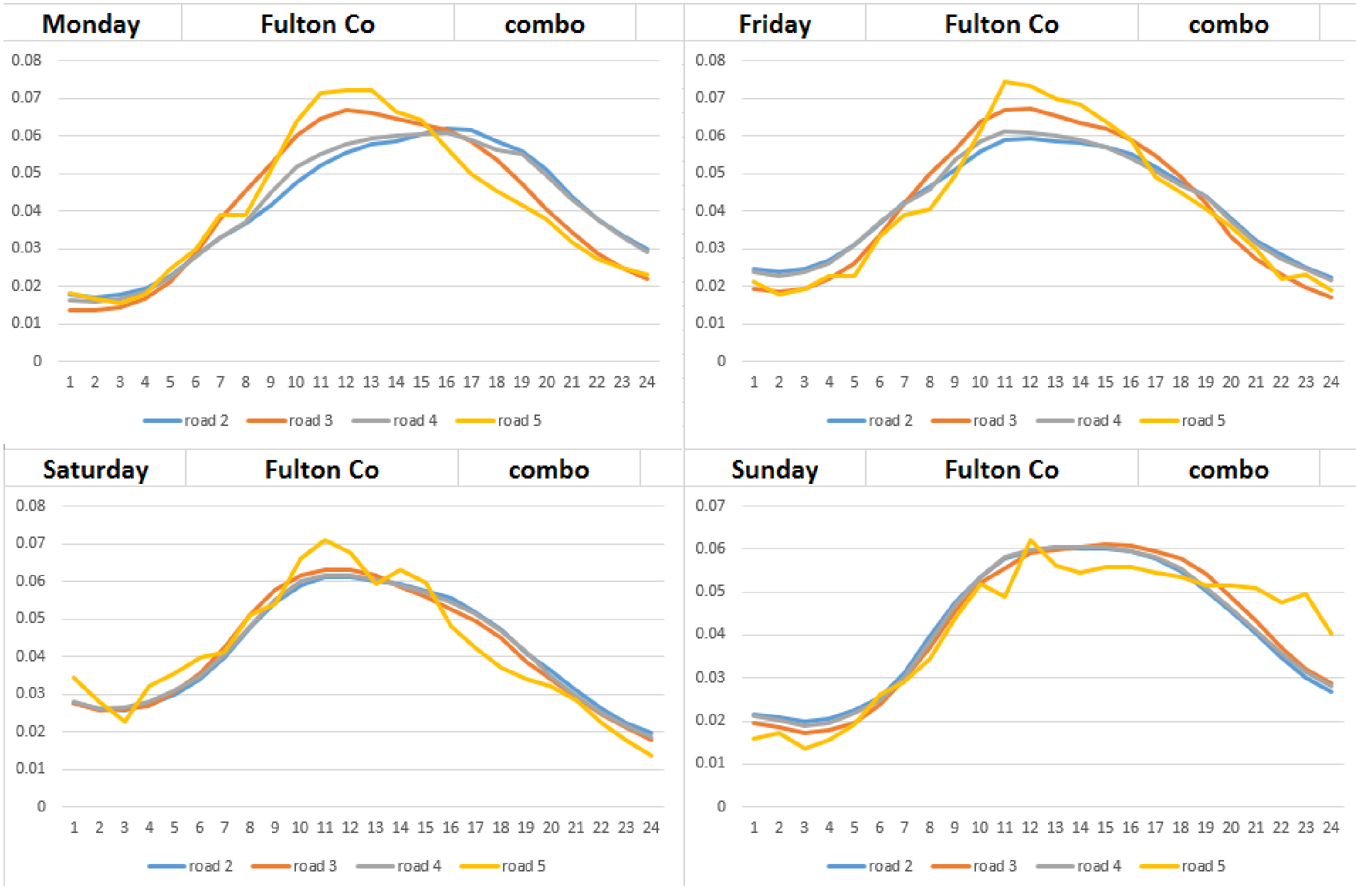


For hoteling, day-of-week profiles are the same as non-hoteling for combination trucks, while hour-of-day non-hoteling profiles for combination trucks were inverted to create new hoteling profiles that peak overnight instead of during the day. The combination truck profiles for Fulton County are shown in Figure 3-20.

The CRC A-100 temporal profiles were used in the entire contiguous United States, except in California. All California temporal profiles were carried over from 2014v7.0, although California hoteling uses CRC A-100-based profiles just like the rest of the country, since CARB didn't have a hoteling-specific profile. Monthly profiles in all states (national profiles by broad vehicle type) were also carried over from 2014v7.0 and applied directly to the VMT. For California, CARB supplied diurnal profiles that varied by vehicle type, day of the week[13], 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.

[13] 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 3-20. 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.

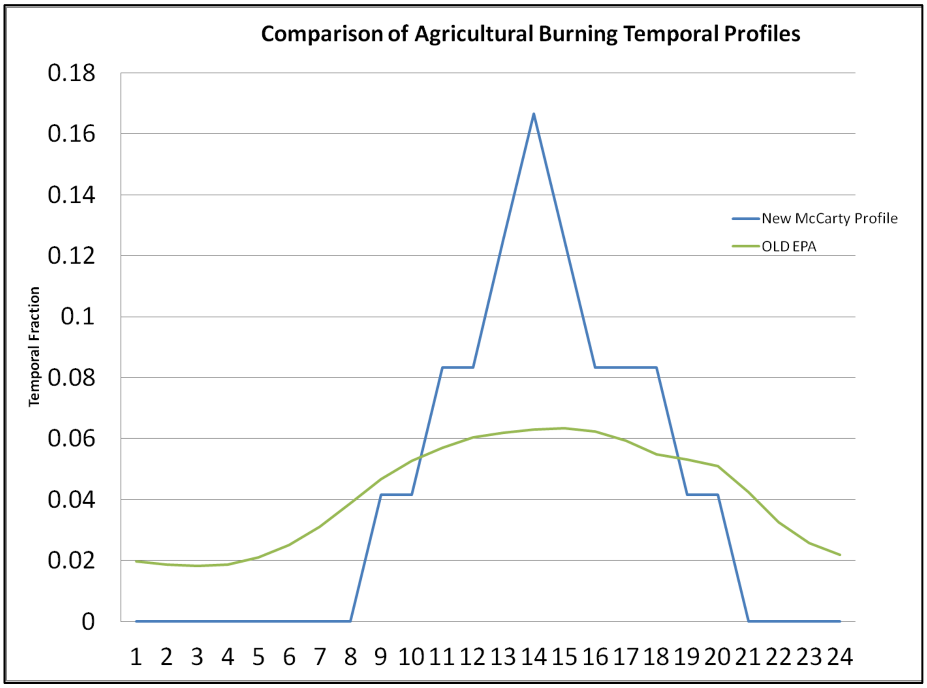
Biogenic emissions in the beis sector vary by every day of the year because they are developed using meteorological data including temperature, surface pressure, and radiation/cloud data. The emissions are computed using appropriate emission factors according to the vegetation in each model grid cell, 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 NOx emissions were normalized to create temporal profiles for each lake. For the port SCCs, an in-port profile was developed as the average of the maneuvering and hoteling emissions. The cruising emissions were used for the underway SCCs. As some of the lakes did not include complete data for the in-port sources (Ontario, Canada, St. Claire), a hybrid profile was created as an average of the in-port NOx emissions for Lakes Michigan, Huron, Superior, and Erie. A resulting 22 profiles were developed and applied to C1, C2 and C3 ships based county and SCC (i.e., port versus underway). Only new monthly profiles were developed from these data because the weekly and diurnal variation were deemed to be comparable to the existing EPA profiles. For non-LADCO areas, C1 and C2 monthly profiles are flat and C3 monthly profiles are highest (but not significantly different from the rest of the year) in the summer.

For the rail sector, new monthly profiles were developed for the 2016 platform. Monthly temporal allocation for rail freight emissions is based on AAR Rail Traffic Data, Total Carloads and Intermodal, for 2016. For passenger trains, monthly temporal allocation is flat for all months. Rail passenger miles data is available by month for 2016 but it is not known how closely rail emissions track with passenger activity since passenger trains run on a fixed schedule regardless of how many passengers are aboard, and so a flat profile is chosen for passenger trains. Rail emissions are allocated with flat day of week profiles, and most emissions are allocated with flat hourly profiles.

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 3-21 (McCarty et al., 2009). This puts most of the emissions during the work day and suppresses the emissions during the middle of the night.

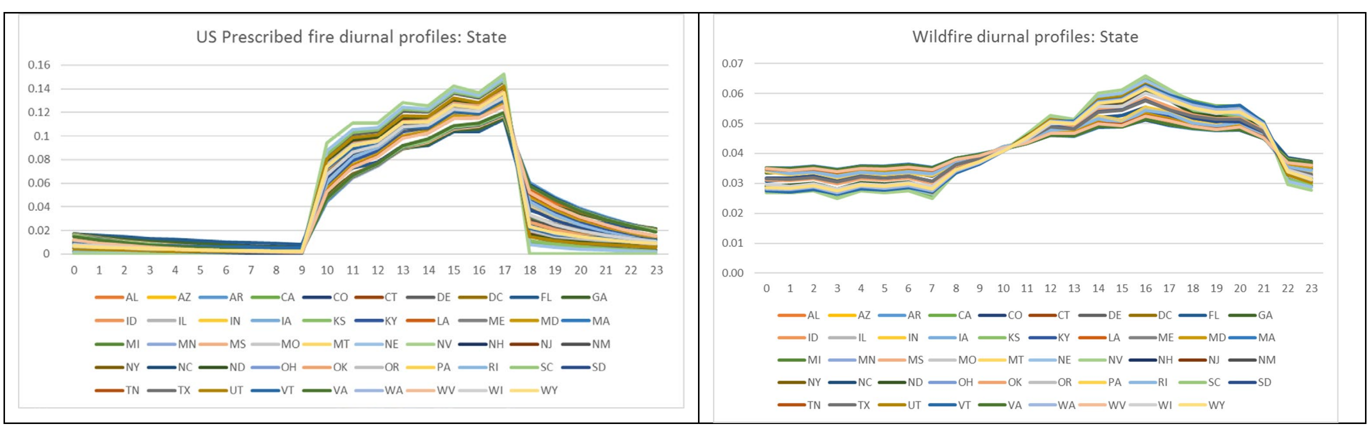
Figure 3-21. Agricultural burning diurnal temporal profile



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 3-22 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 form 2014v7.1 platform.

Figure 3-22. 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 national 36-km and 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 the 2016v7.2 platform. 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 3-20 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 the 2016v7.1 (aka 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.

In addition, spatial surrogates 201 through 244, which concern road miles, annual average daily traffic (AADT), and truck stops, were further updated for the 2016 beta and regional haze platforms. 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 3-20. U.S. Surrogates available for the 2016 alpha and beta modeling platforms

Code	Surrogate Description	Code	Surrogate Description
N/A	Area-to-point approach (see 3.6.2)	505	Industrial Land
100	Population	506	Education
110	*Housing*	*507*	*Heavy Light Construction Industrial Land*
131	*urban Housing*	*510*	*Commercial plus Industrial*
132	*Suburban Housing*	*515*	*Commercial plus Institutional Land*
134	*Rural Housing*	*520*	*Commercial plus Industrial plus Institutional*
137	*Housing Change*	*525*	*Golf Courses plus Institutional plus Industrial plus Commercial*
140	*Housing Change and Population*	*526*	*Residential – Non-Institutional*
150	Residential Heating – Natural Gas	*527*	*Single Family Residential*
160	*Residential Heating – Wood*	535	Residential + Commercial + Industrial + Institutional + Government
170	Residential Heating – Distillate Oil	*540*	*Retail Trade (COM1)*
180	Residential Heating – Coal	*545*	*Personal Repair (COM3)*
190	Residential Heating – LP Gas	*555*	*Professional/Technical (COM4) plus General Government (GOV1)*
201	*Urban Restricted Road Miles*	560	Hospital (COM6)
202	Urban Restricted AADT	*575*	*Light and High Tech Industrial (IND2 + IND5)*
205	Extended Idle Locations	*580*	*Food Drug Chemical Industrial (IND3)*
211	*Rural Restricted Road Miles*	*585*	*Metals and Minerals Industrial (IND4)*
212	*Rural Restricted AADT*	*590*	*Heavy Industrial (IND1)*
221	*Urban Unrestricted Road Miles*	*595*	*Light Industrial (IND2)*
222	*Urban Unrestricted AADT*	*596*	*Industrial plus Institutional plus Hospitals*
231	*Rural Unrestricted Road Miles*	650	Refineries and Tank Farms
232	*Rural Unrestricted AADT*	670	Spud Count – CBM Wells
239	Total Road AADT	671	Spud Count – Gas Wells
240	Total Road Miles	672	Gas Production at Oil Wells
241	*Total Restricted Road Miles*	673	Oil Production at CBM Wells
242	All Restricted AADT	674	Unconventional Well Completion Counts
243	*Total Unrestricted Road Miles*	*676*	*Well Count – All Producing*
244	All Unrestricted AADT	*677*	*Well Count – All Exploratory*
258	Intercity Bus Terminals	678	Completions at Gas Wells
259	Transit Bus Terminals	679	Completions at CBM Wells
260	*Total Railroad Miles*	681	Spud Count – Oil Wells
261	NTAD Total Railroad Density	683	Produced Water at All Wells

Code	Surrogate Description	Code	Surrogate Description
271	NTAD Class 1 2 3 Railroad Density	685	Completions at Oil Wells
272	*NTAD Amtrak Railroad Density*	*686*	*Completions at All Wells*
273	*NTAD Commuter Railroad Density*	687	Feet Drilled at All Wells
275	*ERTAC Rail Yards*	691	Well Counts - CBM Wells
280	*Class 2 and 3 Railroad Miles*	692	Spud Count – All Wells
300	NLCD Low Intensity Development	693	Well Count – All Wells
301	*NLCD Med Intensity Development*	694	Oil Production at Oil Wells
302	*NLCD High Intensity Development*	695	Well Count – Oil Wells
303	*NLCD Open Space*	696	Gas Production at Gas Wells
304	NLCD Open + Low	697	Oil Production at Gas Wells
305	NLCD Low + Med	698	Well Count – Gas Wells
306	NLCD Med + High	699	Gas Production at CBM Wells
307	NLCD All Development	*710*	*Airport Points*
308	NLCD Low + Med + High	711	Airport Areas
309	NLCD Open + Low + Med	801	Port Areas
310	NLCD Total Agriculture	*805*	*Offshore Shipping Area*
318	*NLCD Pasture Land*	*806*	*Offshore Shipping NEI2014 Activity*
319	NLCD Crop Land	*807*	*Navigable Waterway Miles*
320	NLCD Forest Land	808	2013 Shipping Density
321	NLCD Recreational Land	820	Ports NEI2014 Activity
340	*NLCD Land*	850	Golf Courses
350	NLCD Water	860	Mines
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 3-21. 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 2016 platforms to include additional data sources and corrections based on comments received.

Table 3-21. 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 3-22 using 2016 data consistent with what was used to develop the 2016 beta 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, 2017). 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 2016. 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 3-22. 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 3-20 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 3-23 shows the CAP emissions (i.e., NH_3, NOx, $PM_{2.5}$, SO_2, and VOC) by sector assigned to each spatial surrogate.

Table 3-23. Selected 2016 CAP emissions by sector for U.S. Surrogates (short tons in 12US1)

Sector	ID	Description	NH3	NOX	PM2_5	SO2	VOC
afdust	240	Total Road Miles	--	--	295,442	--	--
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	2,856,742	--	--	--	186,274
cmv_c1c2	808	2013 Shipping Density	297	489,917	12,963	1,736	8,543
cmv_c1c2	820	Ports NEI2014 Activity	11	23,996	735	1,386	985
nonpt	100	Population	32,842	0	0	0	1,244,799
nonpt	150	Residential Heating - Natural Gas	47,820	227,295	3,837	1,494	13,757
nonpt	170	Residential Heating - Distillate Oil	1,865	35,187	3,988	56,230	1,245
nonpt	180	Residential Heating - Coal	20	101	53	1,086	111
nonpt	190	Residential Heating - LP Gas	121	34,439	183	762	1,332
nonpt	239	Total Road AADT	0	25	551	0	274,991
nonpt	240	Total Road Miles	0	0	0	0	34,042
nonpt	242	All Restricted AADT	0	0	0	0	5,451
nonpt	244	All Unrestricted AADT	0	0	0	0	95,312
nonpt	271	NTAD Class 1 2 3 Railroad Density	0	0	0	0	2,252
nonpt	300	NLCD Low Intensity Development	5,198	27,749	104,168	3,725	75,096
nonpt	306	NLCD Med + High	28,101	200,139	240,282	64,743	955,021
nonpt	307	NLCD All Development	25	46,372	126,828	14,199	602,300
nonpt	308	NLCD Low + Med + High	1,134	185,338	16,837	18,989	65,604
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	99,043
nonpt	711	Airport Areas	0	0	0	0	287
nonpt	801	Port Areas	0	0	0	0	8,059
nonroad	261	NTAD Total Railroad Density	3	2,157	222	2	431
nonroad	304	NLCD Open + Low	4	1,836	159	5	2,988
nonroad	305	NLCD Low + Med	95	16,298	3,866	129	116,725

Sector	ID	Description	NH3	NOX	PM2_5	SO2	VOC
nonroad	306	NLCD Med + High	306	184,311	11,935	426	96,119
nonroad	307	NLCD All Development	107	33,798	16,275	135	178,932
nonroad	308	NLCD Low + Med + High	491	340,485	29,187	510	53,506
nonroad	309	NLCD Open + Low + Med	131	22,947	1,367	178	49,881
nonroad	310	NLCD Total Agriculture	366	347,896	25,991	408	38,673
nonroad	320	NLCD Forest Land	15	6,020	674	15	3,666
nonroad	321	NLCD Recreational Land	83	11,923	6,353	139	243,437
nonroad	350	NLCD Water	184	121,152	6,929	248	365,285
nonroad	850	Golf Courses	13	2,052	119	18	5,704
nonroad	860	Mines	2	2,698	281	3	522
np_oilgas	670	Spud Count - CBM Wells	0	0	0	0	113
np_oilgas	671	Spud Count - Gas Wells	0	0	0	0	6,768
np_oilgas	674	Unconventional Well Completion Counts	12	19,127	731	9	1,284
np_oilgas	678	Completions at Gas Wells	0	274	0	6,743	32,577
np_oilgas	679	Completions at CBM Wells	0	3	0	80	395
np_oilgas	681	Spud Count - Oil Wells	0	0	0	0	16,718
np_oilgas	683	Produced Water at All Wells	0	11	0	0	47,204
np_oilgas	685	Completions at Oil Wells	0	254	0	763	27,822
np_oilgas	687	Feet Drilled at All Wells	0	38,373	1,391	27	2,785
np_oilgas	691	Well Counts - CBM Wells	0	32,341	481	12	27,342
np_oilgas	692	Spud Count - All Wells	0	8,884	253	99	353
np_oilgas	693	Well Count - All Wells	0	0	0	0	159
np_oilgas	694	Oil Production at Oil Wells	0	4,165	0	15,385	1,060,803
np_oilgas	695	Well Count - Oil Wells	0	143,918	3,099	34	600,255
np_oilgas	696	Gas Production at Gas Wells	0	16,562	1,871	166	431,037
np_oilgas	698	Well Count - Gas Wells	0	298,879	6,173	248	645,169
np_oilgas	699	Gas Production at CBM Wells	0	2,413	312	25	7,612
onroad	205	Extended Idle Locations	499	177,484	2,129	72	32,817
onroad	239	Total Road AADT	0	0	0	0	6,021
onroad	242	All Restricted AADT	35,855	1,316,007	41,161	8,564	205,314
onroad	244	All Unrestricted AADT	64,487	1,929,809	75,033	17,881	517,975
onroad	258	Intercity Bus Terminals	0	141	2	0	31
onroad	259	Transit Bus Terminals	0	82	4	0	180
onroad	304	NLCD Open + Low	0	762	17	1	2,698
onroad	306	NLCD Med + High	0	15,478	283	18	17,706
onroad	307	NLCD All Development	0	584,068	11,221	945	1,142,084
onroad	308	NLCD Low + Med + High	0	41,226	698	64	60,234
rail	261	NTAD Total Railroad Density	15	33,822	1051	16	1626
rail	271	NTAD Class 1 2 3 Railroad Density	307	523,394	15,063	346	24,365
rwc	300	NLCD Low Intensity Development	15,491	31,432	318,099	7,929	417,395

For 36US3 modeling in the 2016 alpha and beta / regional haze platforms, 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). 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). 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 Mexico municipio level emissions have been updated in the 2014v7.1 platform and carried forward into the 2016 alpha platform. For the 2016v7.2 platform, a new set of Canada shapefiles were provided by Environment Canada along with cross references spatially allocate the year 2015 Canadian emissions. Gridded surrogates were generated using the Surrogate Tool (previously referenced); Table 3-24 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 3-25.

Table 3-24. Canadian Spatial Surrogates

Code	Canadian Surrogate Description	Code	Description
100	Population	923	TOTAL INSTITUTIONAL AND GOVERNEMNT
101	total dwelling	924	Primary Industry
104	capped total dwelling	925	Manufacturing and Assembly

Code	Canadian Surrogate Description	Code	Description
106	ALL_INDUST	926	Distribtution and Retail (no petroleum)
113	Forestry and logging	927	Commercial Services
200	Urban Primary Road Miles	932	CANRAIL
210	Rural Primary Road Miles	940	PAVED ROADS NEW
211	Oil and Gas Extraction	945	Commercial Marine Vessels
212	Mining except oil and gas	946	Construction and mining
220	Urban Secondary Road Miles	948	Forest
221	Total Mining	951	Wood Consumption Percentage
222	Utilities	955	UNPAVED_ROADS_AND_TRAILS
230	Rural Secondary Road Miles	960	TOTBEEF
233	Total Land Development	970	TOTPOUL
240	capped population	980	TOTSWIN
308	Food manufacturing	990	TOTFERT
321	Wood product manufacturing	996	urban_area
323	Printing and related support activities	1251	OFFR_TOTFERT
324	Petroleum and coal products manufacturing	1252	OFFR_MINES
326	Plastics and rubber products manufacturing	1253	OFFR Other Construction not Urban
327	Non-metallic mineral product manufacturing	1254	OFFR Commercial Services
331	Primary Metal Manufacturing	1255	OFFR Oil Sands Mines
350	Water	1256	OFFR Wood industries CANVEC
412	Petroleum product wholesaler-distributors	1257	OFFR UNPAVED ROADS RURAL
448	clothing and clothing accessories stores	1258	OFFR_Utilities
482	Rail transportation	1259	OFFR total dwelling
562	Waste management and remediation services	1260	OFFR_water
901	AIRPORT	1261	OFFR_ALL_INDUST
902	Military LTO	1262	OFFR Oil and Gas Extraction
903	Commercial LTO	1263	OFFR_ALLROADS
904	General Aviation LTO	1265	OFFR_CANRAIL
921	Commercial Fuel Combustion	9450	Commercial Marine Vessel Ports

Table 3-25. CAPs Allocated to Mexican and Canadian Spatial Surrogates (short tons in 36US3)

Sector	Code	Mexican or Canadian Surrogate Description	NH_3	NO_X	PM_{2_5}	SO_2	VOC
othafdust	106	CAN ALL_INDUST	--	--	5,632	--	--
othafdust	212	CAN Mining except oil and gas	--	--	684	--	--
othafdust	221	CAN Total Mining	--	--	142,940	--	--
othafdust	222	CAN Utilities	--	--	23,640	--	--
othafdust	940	CAN Paved Roads New	--	--	210,336	--	--
othafdust	955	CAN UNPAVED_ROADS_AND_TRAILS	--	--	389,775	--	--
othafdust	960	CAN TOTBEEF	--	--	1,289	--	--
othafdust	970	CAN TOTPOUL	--	--	184	--	--
othafdust	980	CAN TOTSWIN	--	--	792	--	--
othafdust	990	CAN TOTFERT	--	--	321	--	--
othafdust	996	CAN urban_area	--	--	617	--	--
othar	11	MEX 2015 Population	164,464	168,447	13,521	1,164	291,178

Sector	Code	Mexican or Canadian Surrogate Description	NH_3	NO_X	PM $_{2\_5}$	SO_2	VOC
othar	14	MEX Residential Heating - Wood	0	23,842	305,597	3,658	2,101,033
othar	16	MEX Residential Heating - Distillate Oil	2	58	1	16	2
othar	20	MEX Residential Heating - LP Gas	0	26,526	838	0	505
othar	22	MEX Total Road Miles	1	1,046	2	7	2,308
othar	24	MEX Total Railroads Miles	0	63,136	1,407	551	2,494
othar	26	MEX Total Agriculture	713,253	399,070	80,458	18,650	33,742
othar	32	MEX Commercial Land	0	457	7,719	0	106,077
othar	34	MEX Industrial Land	8	3,383	4,833	1	563,953
othar	36	MEX Commercial plus Industrial Land	0	0	0	0	272,155
othar	38	MEX Commercial plus Institutional Land	3	6,740	235	3	148
othar	40	MEX Residential (RES1-4)+Commercial+ Industrial+Institutional+Government	0	16	39	0	331,216
othar	42	MEX Personal Repair (COM3)	0	0	0	0	26,261
othar	44	MEX Airports Area	0	13,429	306	1,561	3,766
othar	50	MEX Mobile sources - Border Crossing	5	161	1	3	293
othar	100	CAN Population	761	54	669	15	241
othar	101	CAN total dwelling	0	0	0	0	150,892
othar	104	CAN Capped Total Dwelling	421	37,205	2,766	206	1,952
othar	113	CAN Forestry and logging	185	2,210	11,310	45	6,246
othar	211	CAN Oil and Gas Extraction	0	31	60	22	925
othar	212	CAN Mining except oil and gas	0	0	3,079	0	0
othar	221	CAN Total Mining	0	0	43	0	0
othar	222	CAN Utilities	34	1,858	0	386	22
othar	308	CAN Food manufacturing	0	0	20,185	0	10,324
othar	321	CAN Wood product manufacturing	874	4,822	1,646	383	16,606
othar	323	CAN Printing and related support activities	0	0	0	0	11,770
othar	324	CAN Petroleum and coal products manufacturing	0	1,205	1,542	486	9,304
othar	326	CAN Plastics and rubber products manufacturing	0	0	0	0	23,283
othar	327	CAN Non-metallic mineral product manufacturing	0	0	6,695	0	0
othar	331	CAN Primary Metal Manufacturing	0	158	5,595	30	72
othar	350	CAN Water	0	120	2	0	4
othar	412	CAN Petroleum product wholesaler-distributors	0	0	0	0	45,257
othar	448	CAN clothing and clothing accessories stores	0	0	0	0	149
othar	482	CAN Rail Transportation	2	4,980	106	12	310
othar	562	CAN Waste management and remediation services	271	1,977	2,710	2,528	13,138
othar	901	CAN Airport	0	109	11	0	11
othar	921	CAN Commercial Fuel Combustion	243	23,628	2,333	2,821	1,091
othar	923	CAN TOTAL INSTITUTIONAL AND GOVERNEMNT	0	0	0	0	14,859
othar	924	CAN Primary Industry	0	0	0	0	40,376
othar	925	CAN Manufacturing and Assembly	0	0	0	0	71,198
othar	926	CAN Distribtution and Retail (no petroleum)	0	0	0	0	7,461
othar	927	CAN Commercial Services	0	0	0	0	32,167
othar	932	CAN CANRAIL	61	132,985	3,107	485	6,567
othar	945	CAN Commercial Marine Vessels	69	53,264	966	549	2,659

Sector	Code	Mexican or Canadian Surrogate Description	NH_3	NO_X	PM_{2_5}	SO_2	VOC
othar	946	CAN Construction and Mining	0	0	0	0	4,359
othar	951	CAN Wood Consumption Percentage	1,950	21,662	179,087	3,095	253,523
othar	990	CAN TOTFERT	48	4,456	0	9,881	164
othar	1251	CAN OFFR_TOTFERT	81	77,166	5,671	58	7,176
othar	1252	CAN OFFR_MINES	1	1,004	70	1	138
othar	1253	CAN OFFR Other Construction not Urban	66	53,671	6,096	47	12,159
othar	1254	CAN OFFR Commercial Services	40	17,791	2,552	34	44,338
othar	1255	CAN OFFR Oil Sands Mines	18	9,491	311	10	1,025
othar	1256	CAN OFFR Wood industries CANVEC	9	5,856	476	7	1,318
othar	1257	CAN OFFR Unpaved Roads Rural	32	11,866	1,169	28	49,975
othar	1258	CAN OFFR_Utilities	8	5,579	349	7	1,087
othar	1259	CAN OFFR total dwelling	16	5,768	773	14	15,653
othar	1260	CAN OFFR_water	15	4,356	451	29	28,411
othar	1261	CAN OFFR_ALL_INDUST	4	5,770	253	3	1,049
othar	1262	CAN OFFR Oil and Gas Extraction	0	368	29	0	143
othar	1263	CAN OFFR_ALLROADS	3	2,418	244	2	582
othar	1265	CAN OFFR_CANRAIL	0	85	9	0	15
othar	9450	CAN Commercial Marine Ports	1	5,690	148	473	199
onroad_can	200	CAN Urban Primary Road Miles	1,619	85,558	2,851	329	8,396
onroad_can	210	CAN Rural Primary Road Miles	683	51,307	1,673	139	3,807
onroad_can	220	CAN Urban Secondary Road Miles	3,021	136,582	5,708	690	22,374
onroad_can	230	CAN Rural Secondary Road Miles	1,769	96,911	3,238	374	10,370
onroad_can	240	CAN Total Road Miles	43	57,401	1,355	77	103,658
onroad_mex	11	MEX 2015 Population	0	281,317	1,873	533	291,992
onroad_mex	22	MEX Total Road Miles	10,321	1,208,461	54,823	25,855	251,931
onroad_mex	36	MEX Commercial plus Industrial Land	0	7,975	142	29	9,192

3.5 Preparation of Emissions for the CAMx model

3.5.1 Development of CAMx Emissions for Standard CAMx Runs

For this study, we perform air quality modeling with the Comprehensive Air Quality Model with Extensions (CAMx model). Gridded hourly emissions output by the SMOKE model are output in the format needed by 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. For "regular" CAMx modeling (i.e., without two-way nesting), 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 (24^{th}) hour of a CAMx-ready emissions file will equal the average of the last two hours (24^{th} and 25^{th}) 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 (PM2.5), and other model species, is provided in Table 3-26. 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 3-26.

Table 3-26. 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
	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

Inventory Pollutant	CMAQ Model Species	CAMx Model Species
	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 ocean chlorine emissions. 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 (i.e., sea salt).

3.5.2 Development of CAMx Emissions for Two-Way Nested CAMx Runs in This Study

Version 7 of the CAMx model supports a new type of modeling called two-way nested modeling. In a standard model run, CAMx is run for the 36US3 grid first, and then run a second time for the 12US2 grid using boundary conditions derived from the 36US3 run. In a two-way nested model run, CAMx is run for both the 36US3 and 12US2 grids at the same time with feedback between the domains, eliminating the need for two separate model runs. CAMx modeling for this study was performed using the two-way nesting feature.

For a regular CAMx model run, two emissions files per day are provided to the model: a gridded file of low-level emissions (the “emis2d” file), and a file of point source emissions (the “mrgpt” file). For a two-way nested CAMx model run, we provide two emis2d files per day; one for the 36US3 domain, and one for the “12US2b” domain, not for the 12US2 domain as described below. A single mrgpt file is provided to the model which covers all sources in the 36US3 domain. For all point sources except fires, the mrgpt file has location and stack information for individual sources, and so for all point sources except fires, a point source file developed for the 36US3 domain can be used for 12US2 modeling without losing resolution.

For the ptfire, ptagfire, and ptfire_othna sectors, support for two-way nested modeling requires additional emissions modeling considerations. Fire emissions are unique from other point sectors in that CAMx modeling does not support inline plume rise for fires, and so we calculate plume rise for fires within SMOKE as described in the prior section. As part of calculating plume rise, it is necessary for the emissions to be gridded by SMOKE as well. Therefore, layered fire emissions files for the 36US3 domain output by SMOKE only have 36km resolution, and as such we cannot simply merge the 36US3 fire emissions in the mrgpt file like we can for other point sectors, or else the fire emissions within the 12US2 domain will have 36km resolution. To support two-way nested modeling, we need the mrgpt file to include fire emissions with 12km resolution in the area covered by the 12US2 domain, and 36km resolution in the area outside of the 12US2 domain. To account for this, the following fire emissions are included in the mrgpt file:

- Layered 12US2 emissions for the ptfire, ptagfire, and ptfire_othna sectors
- Layered 36US3 emissions for the ptfire_othna sector, but with the region of the domain which overlaps 12US2 zeroed out to avoid a double count
- Layered 36US3 emissions for the Southeast Alaska portion of the ptfire sector (which only exist on two days in 2016; ptagfire does not have any Southeast Alaska emissions)

Development of the emis2d files for two-way nested modeling is the same as for regular modeling, with one exception: to support two-way nested modeling, the 12US2 emis2d file must have an extra row and column of cells added to each edge of the domain, expanding the size of the domain by two rows and two columns. The resulting 12km-resolution domain with two extra rows and columns is referred to as the 12US2b domain. The CAMx model requires these extra rows and columns to facilitate feedback between the two domains. The emissions values in the extra rows and columns do not affect the model results, and so it is not necessary to consider the 12US2b domain throughout the emissions modeling process. In other words, it is valid to process emissions for 12US2, same as for a regular model run, and then convert the 12US2 emissions to the 12US2b domain in the last step. We do this with a utility which adds a row and column to the edge of the domain, with zero emissions for all species in the extra rows and columns.

3.5.3 Development of CAMx Emissions for Source Apportionment CAMx Runs

The CAMx model supports source apportionment modeling for PM sources, using a technique called Particulate Matter Source Apportionment Technology (PSAT). PSAT allows emissions from different types of sources to be tracked through the CAMx model. For this study, PSAT modeling was performed in CAMx with two-way nesting for the 2028, and a new set of emissions was developed specifically for PSAT modeling with the case name “2028fg_secsa_16j”.

Source Apportionment modeling involves assigning tags to different categories of emissions. These tags can be applied by region (e.g. state), by emissions type (e.g. SCC or sector), or a combination of the two. For this study, emissions tagging was applied by sector, as shown in Table 3-27.

Table 3-27. Sector tags for 2028fg PSAT modeling

tag	emissions applied to tag
1	All biogenics (beis sector)
2	US EGUs (ptegu sector)
3	US onroad (onroad and onroad_ca_adj sectors)
4	US nonroad (nonroad sector)
5	US CMV C1/C2, including Federal Waters (cmv_c1c2 sector)
6	US CMV C3 in state and federal waters (cmv_c3 sector, except for FIPS 98001)
7	CMV C3 outside US and Canada federal waters (cmv_c3 sector, FIPS 98001 only)
8	US rail (rail sector)
9	US ag fires (ptagfire sector)
10	US agriculture (ag sector)
11	US oil and gas (np_oilgas and pt_oilgas sectors)
12	US non-EGU point, including airports and rail yards (ptnonipm sector)
13	US residential wood combustion (rwc sector)
14	US wildfires (part of ptfire sector)
15	US prescribed fires (part of ptfire sector)
16	US fugitive dust (afdust_adj sector)
17	US other nonpoint (nonpt sector)
18	Canada fires (part of ptfire_othna sector)
19	Canada anthropogenics (part of othar and othpt sectors, plus all of onroad_can, othafdust_adj, and othptdust_adj)
20	Mexico fires (part of ptfire_othna sector)
21	Mexico anthropogenics (part of othar and othpt sectors, plus all of onroad_mex)
22	Oceanic sea salt (sulfate)
1BC	Boundary Conditions – International Anthropogenic
1IC	Initial Conditions – International Anthropogenic
2BC	Boundary Conditions – Natural
2IC	Initial Conditions – other
TOPCON	Top Concentrations

For PSAT modeling, all emissions must be input to CAMx in the form of a point source (mrgpt) file, including low level sources. In addition, for two-way nested modeling, all emissions must be input in a *single* mrgpt file, rather than separate mrgpt files for each of the two domains (36US3 and 12US2). As described above, fire emissions require special consideration in two-way nested model runs; for PSAT modeling, that same consideration must be given to any sector in which emissions are being gridded by SMOKE.

There are two main approaches for tagging emissions for CAMx modeling. One approach is to tag emissions within SMOKE. Here, SMOKE will output tagged point source files (SGINLN files), which can then be converted to CAMx point source format with the tags applied by SMOKE carried forward into the CAMx inputs. The second approach is to, if necessary depending on the nature of the tags, split sectors into multiple components by tag so that each sector corresponds to a single tag. Then, the gridded and/or point source format SMOKE outputs from those split sectors are converted to CAMx point source format, and then merged into the full mrgpt file, with the tags applied at that last step. Development of the 2028fg_secsa_16j emissions includes a mix of the two approaches.

For most sectors, the second approach was used, meaning SMOKE is run normally with sectors split into multiple parts if necessary, and with the SMOKE outputs converted to point source format and then tagged on the back end. Two-way nested modeling requires additional considerations to ensure that, like with fire emissions in a non-PSAT CAMx model run, gridded emissions have 12km resolution in the 12US2 area and 36km resolution elsewhere. Sectors that were processed and tagged this way include:

- For ag (10), np_oilgas (11), onroad_ca_adj (3), ptagfire (9), rail (8), ptegu (2): These sectors have a single tag and do not have any emissions which lie outside the 12US2 domain and inside the 36US3 domain (which as far as the US is concerned, only includes Southeast Alaska). So, the gridded 12US2 emissions from the regular 2028fg run were used and a sector-wide tag applied.

- For afdust (16), onroad (3): These sectors have a single tag, but do have some Southeast Alaska emissions in the 36US3 domain. Since the 36US3 emissions are derived from 12US2, the Alaska emissions are already processed separately under the sector names afdust_ak_adj and onroad_nonconus. The 12US2 afdust_adj and onroad emissions are converted to CAMx format with sector-wide tags applied. Then, the 36US3 Alaska-only afdust_ak_adj and onroad_nonconus emissions are converted to CAMx format with the same sector-wide tags applied.

- For nonpt (17), nonroad (4), rwc (13): These sectors have a single tag, but do have some Southeast Alaska emissions in 36US3. Thus, a second set of 36US3 emissions was created for these sectors that only include Alaska. Then, the 36US3 Alaska-only files and full 12US2 files are each converted to CAMx format with sector-wide tags applied.

- For beis (1), cmv_c1c2 (5), onroad_can (19), onroad_mex (21), othafdust (19), othptdust (19), sea salt (22): These sectors have a single tag, and also have emissions that exist beyond the boundaries of 12US2. Thus, a second set of 36US3 emissions was created for these sectors that has the portion of the domain which overlaps 12US2 zeroed out, or "masked". Then, the masked 36US3 emissions and and full 12US2 files are each converted to CAMx format with sector-wide tags applied.

- For ptfire (14/15), ptfire_othna (18/20): These are layered fire sectors, each with two tags, and each with emissions outside of 12US2. (The ptfire does have some emissions in Southeast Alaska.) For these sectors, the procedure is: 1) Split the sector into two parts, one part per tag. The ptfire inventory is split into a wildfire component and a prescribed component, and the ptfire_othna inventory is split into Canada and Mexico components. 2) Process each component through SMOKE separately for both 36US3 and 12US2, with layering. 3) Mask the 12US2 portion out of the 36US3 gridded and layered emissions. 4) Convert full 12US2 + masked 36US3 to CAMx format, preserving layering.

- For othar: This sector has two tags (Canada 19, Mexico 21). The procedure is the same as for ptfire and ptfire_othna, except without layering.

The cmv_c3 and othpt sectors were processed with the SGINLN approach using a tagging file applied by SMOKE. The cmv_c3 and othpt sectors have two tags each, applied within SMOKE. Since these are point sectors which are not gridded by SMOKE, the sectors only needed to be processed for the 36US3 domain without special consideration for two-way nesting.

The ptnonipm and pt_oilgas sectors are also point sectors that required special consideration for two-way nesting when tagging. These sectors are normally processed through SMOKE as partially elevated sectors, in which some sources are output to the inline point source file and other sources, depending on stack parameters, are output to a gridded file. When creating SGINLN files for these sectors, sources which would otherwise be output to the gridded file are also gridded in the SGINLN file. In other words, the SGINLN file includes individual point source information for all elevated sources, but includes gridded emissions for low-level sources. This means that unless every source in the sector is considered an elevated source - which is normally the case in cmv_c3 and othpt, but not in ptnonipm and pt_oilgas - a 36US3 SGINLN file cannot be used for two-way nested modeling because the low-level sources in that file will only have 36km resolution. To resolve this for the 2028fg_secsa_16j emissions, the ptnonipm and pt_oilgas sectors were reprocessed through SMOKE with all sources classified as elevated, so that the resulting point source files would retain information for every point source in the sector rather than put the low-level sources on a 36km grid.

Point source files for all of the sectors listed above are then merged together to create the mrgpt file for PSAT modeling which includes all emissions, with the appropriate tags and appropriate resolution throughout the domain.

4 Emission Summaries

Tables 4-1 through 4-4 summarize emissions by sector for the 2016fg and 2028fg cases. These summaries are 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 and for the 36-km domain (36US3). Note that totals for the 12US2 domain are not available here, but the sum of the U.S. sectors would be essentially the same, only the Canadian and Mexican emissions would change according to how far north/south the grids go. Note that the afdust sector emissions here represent the emissions *after* application of both the land use (transport fraction) and meteorological adjustments; therefore, this sector is called "afdust_adj" in these summaries. The afdust emissions in the 36km domain are smaller than those in the 12km domain due to how the adjustment factors are computed and the size of the grid cells. 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 othar sector. The total of all US sectors is listed as "Con U.S. Total." State totals are available in the reports area on the web and FTP site for the 2016 beta / regional haze platform (https://www.epa.gov/air-emissions-modeling/2016v72-beta-platform) .

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

Sector	CO	NH3	NOX	PM10	PM2_5	SO2	VOC
afdust_adj				7,202,127	1,006,412		
ag		2,856,435					186,273
cmv_c1c2	46,873	120	241,103	5,813	5,521	2,231	4,582
cmv_c3	10,780	25	106,234	1,743	1,516	3,757	4,995
nonpt	2,684,785	121,209	757,079	610,603	498,089	161,064	3,707,237
nonroad	10,881,052	1,794	1,090,157	108,882	103,015	2,209	1,151,547
np_oilgas	740,254	12	565,202	14,398	14,311	23,592	2,908,396
onroad	20,330,093	100,841	4,065,702	272,770	130,564	27,547	1,985,763
ptagfire	278,701	54,442	10,824	41,115	28,632	3,908	18,323
ptfire	14,607,348	254,071	232,294	1,545,802	1,305,341	115,781	3,317,409
ptegu	658,287	23,972	1,290,226	163,956	133,491	1,540,557	33,757
ptnonipm	1,858,717	63,464	1,088,652	404,432	261,146	674,382	815,293
pt_oilgas	167,933	4,338	339,440	11,474	10,974	33,224	127,636
rail	102,881	322	557,216	16,612	16,114	363	25,991
rwc	2,118,074	15,427	31,268	317,334	316,808	7,691	340,812
Con. U.S. Total	**54,485,778**	**3,496,471**	**10,375,397**	**10,717,061**	**3,831,936**	**2,596,307**	**14,628,014**
beis	7,163,806		966,421				42,095,853
CONUS + beis	**61,649,584**	**3,496,471**	**11,341,818**	**10,717,061**	**3,831,936**	**2,596,307**	**56,723,867**
Can./Mex./Offshore							
Sector	**CO**	**NH3**	**NOX**	**PM10**	**PM2_5**	**SO2**	**VOC**
Canada othafdust	--	--	--	1,060,979	187,228	--	--
Canada othar	2,732,048	4,888	437,967	314,303	249,213	20,540	834,379
Canada onroad_can	1,665,792	6,877	404,856	25,204	14,076	1,556	143,213
Canada othpt	1,095,894	503,410	812,630	118,370	49,607	999,725	803,870
Canada othptdust	--	--	--	150,943	55,585	--	--
Canada ptfire_othna	760,345	13,015	16,337	84,366	71,652	6,721	185,224
Mexico othar	241,571	201,994	220,491	115,460	54,294	7,717	522,236
Mexico onroad_mex	1,828,101	2,789	442,410	15,151	10,836	6,247	158,812
Mexico othpt	205,083	5,049	447,675	73,256	57,440	476,079	71,031
Mexico ptfire_othna	384,764	7,466	16,665	45,198	38,354	2,798	131,980
Offshore cmv in Federal waters	99,386	254	715,163	14,061	13,220	12,013	24,428
Offshore cmv outside Federal waters	34,966	0	411,067	34,920	32,119	258,869	14,804
Offshore pt_oilgas	50,052	15	48,691	668	667	502	48,210
Non-US Total	**9,098,003**	**745,757**	**3,973,953**	**2,052,880**	**834,290**	**1,792,766**	**2,938,186**

Table 4-2. National by-sector CAP emissions summaries for the 2028fg case, 12US1 grid

Sector	CO	NH_3	NO_X	PM_{10}	$PM_{2.5}$	SO_2	VOC
afdust_adj	--	--	--	7,252,506	1,017,484	--	--
ag	--	2,983,996	--	--	--	--	197,459
cmv_c1c2	48,461	123	136,359	3,476	3,300	2,076	3,281
cmv_c3	15,518	37	96,783	2,504	2,178	5,392	7,200
nonpt	2,746,495	122,505	760,352	663,580	541,739	118,619	3,925,951
nonroad	11,300,514	2,042	607,236	59,682	55,541	1,551	821,997
np_oilgas	783,413	23	563,116	18,095	17,949	31,120	3,373,183
onroad	10,427,337	83,631	1,353,812	211,037	63,041	11,547	885,883
ptagfire	278,701	54,442	10,824	41,115	28,632	3,908	18,323
ptfire	14,607,348	254,071	232,294	1,545,802	1,305,341	115,781	3,317,409
ptegu	671,029	39,533	804,093	147,663	111,617	878,681	29,823
ptnonipm	1,954,661	64,037	1,142,291	411,104	266,947	640,342	819,452
pt_oilgas	170,020	4,344	316,719	12,656	12,086	40,365	146,288
rail	108,232	339	587,191	17,515	16,990	382	27,395
rwc	2,011,643	14,500	31,894	298,669	298,120	6,679	324,230
Con U.S. Total	**45,123,373**	**3,623,622**	**6,642,964**	**10,685,403**	**3,740,967**	**1,856,443**	**13,897,875**
beis	7,163,806		966,421				42,095,853
CONUS + beis	**52,287,179**	**3,623,622**	**7,609,385**	**10,685,403**	**3,740,967**	**1,856,443**	**55,993,728**
Can./Mex./Offshore							
Canada othafdust	--	--	--	1,267,025	222,026	--	--
Canada othar	2,691,939	4,722	312,959	302,486	222,647	20,151	851,377
Canada onroad_can	1,303,551	5,492	168,631	26,129	9,498	698	60,932
Canada othpt	1,149,091	696,115	565,743	96,966	52,822	861,704	758,931
Canada othptdust	--	--	--	151,271	55,706	--	--
Canada ptfire_othna	760,345	13,015	16,337	84,366	71,652	6,721	185,224
Mexico othar	277,263	200,038	252,523	120,590	58,294	8,206	628,715
Mexico onroad_mex	1,615,412	3,732	393,339	18,728	12,667	8,530	164,793
Mexico othpt	249,257	7,273	499,300	91,716	70,229	433,688	102,109
Mexico ptfire_othna	384,764	7,466	16,665	45,198	38,354	2,798	131,980
Offshore cmv in Federal waters	119,333	285	527,701	13,145	12,141	16,503	31,052
Offshore cmv outside Federal waters	49,724	0	587,745	49,875	45,894	52,793	21,171
Offshore pt_oilgas	50,052	15	48,691	668	667	502	48,210
Non-US Total	**8,650,731**	**938,153**	**3,389,634**	**2,268,163**	**872,597**	**1,412,294**	**2,984,494**

Table 4-3. National by-sector CAP emissions summaries for the 2016fg case, 36US3 grid

Sector	CO	NH3	NOX	PM10	PM2_5	SO2	VOC
afdust_adj				7,204,014	1,006,603		
ag		2,856,435					186,273
cmv_c1c2	48,591	124	249,496	6,016	5,717	2,233	4,675
cmv_c3	11,361	26	112,318	1,821	1,587	3,911	5,254
nonpt	2,686,510	121,265	757,492	610,807	498,233	161,296	3,707,939
nonroad	10,884,434	1,795	1,090,387	108,917	103,048	2,210	1,152,385
np_oilgas	740,254	12	565,202	14,398	14,311	23,592	2,908,396
onroad	20,335,564	100,856	4,066,978	272,851	130,614	27,550	1,986,602
ptagfire	278,701	54,442	10,824	41,115	28,632	3,908	18,323
ptfire	14,607,935	254,081	232,299	1,545,859	1,305,389	115,784	3,317,546
ptegu	658,287	23,972	1,290,226	163,956	133,491	1,540,557	33,757
ptnonipm	1,859,776	63,464	1,088,838	404,485	261,179	674,406	815,393
pt_oilgas	167,933	4,338	339,440	11,474	10,974	33,224	127,636
rail	102,881	322	557,216	16,612	16,114	363	25,991
rwc	2,118,562	15,430	31,277	317,402	316,876	7,692	340,891
Con. U.S. Total	**54,500,788**	**3,496,561**	**10,391,992**	**10,719,726**	**3,832,768**	**2,596,727**	**14,631,060**
beis	7,225,877		969,510				42,184,034
CONUS + beis	**61,726,665**	**3,496,561**	**11,361,502**	**10,719,726**	**3,832,768**	**2,596,727**	**56,815,095**
Can./Mex./Offshore							
Sector	**CO**	**NH3**	**NOX**	**PM10**	**PM2_5**	**SO2**	**VOC**
Canada othafdust				1,101,762	194,352		
Canada othar	2,939,311	5,211	489,313	328,383	261,298	21,337	888,110
Canada onroad_can	1,730,052	7,125	425,462	26,286	14,757	1,606	148,376
Canada othpt	1,329,655	521,321	1,011,385	153,243	59,833	1,124,147	986,821
Canada othptdust				150,113	54,659		
Canada ptfire_othna	6,282,821	104,683	134,301	685,165	580,958	60,914	1,501,988
Mexico othar	2,684,115	878,370	707,975	585,933	415,474	25,671	3,739,965
Mexico onroad_mex	6,273,194	10,319	1,497,028	74,169	56,782	26,400	552,952
Mexico othpt	872,675	36,344	1,043,494	284,434	204,959	2,292,596	356,108
Mexico ptfire_othna	7,136,168	120,627	347,132	1,155,991	746,107	45,222	2,260,695
Offshore cmv in Federal waters	99,782	254	719,270	14,115	13,268	12,115	24,607
Offshore cmv outside Federal waters	88,519	0	1,043,852	88,503	81,432	657,836	37,557
Offshore pt_oilgas	50,052	15	48,691	668	667	502	48,210
Non-US Total	**29,486,344**	**1,684,270**	**7,467,901**	**4,648,763**	**2,684,546**	**4,268,347**	**10,545,391**

Table 4-4. National by-sector CAP emissions summaries for the 2028fg case, 36US3 grid

Sector	CO	NH_3	NO_X	PM_{10}	$PM_{2.5}$	SO_2	VOC
afdust_adj	--	--	--	7,254,396	1,017,675	--	--
ag	--	2,983,996	--	--	--	--	197,459
cmv_c1c2	50,185	127	141,008	3,591	3,411	2,076	3,330
cmv_c3	16,339	39	102,619	2,614	2,278	5,610	7,566
nonpt	2,748,187	122,565	760,786	663,794	541,886	118,858	3,926,655
nonroad	11,303,516	2,043	607,391	59,702	55,559	1,551	822,511
np_oilgas	783,413	23	563,116	18,095	17,949	31,120	3,373,183
onroad	10,429,919	83,643	1,354,242	211,087	63,060	11,549	886,243
ptagfire	278,701	54,442	10,824	41,115	28,632	3,908	18,323
ptfire	14,607,935	254,081	232,299	1,545,859	1,305,389	115,784	3,317,546
ptegu	671,029	39,533	804,093	147,663	111,617	878,681	29,823
ptnonipm	1,955,711	64,037	1,142,485	411,156	266,978	640,367	819,548
pt_oilgas	170,020	4,344	316,719	12,656	12,086	40,365	146,288
rail	108,232	339	587,191	17,515	16,990	382	27,395
rwc	2,012,100	14,503	31,903	298,731	298,182	6,680	324,303
Con U.S. Total	**45,135,286**	**3,623,713**	**6,654,676**	**10,687,972**	**3,741,693**	**1,856,931**	**13,900,174**
beis	7,225,877		969,510				42,184,034
CONUS + beis	**52,361,164**	**3,623,713**	**7,624,186**	**10,687,972**	**3,741,693**	**1,856,931**	**56,084,208**
Can./Mex./Offshore							
Canada othafdust				1,314,491	230,228		
Canada othar	2,902,592	5,034	358,016	314,906	232,768	21,205	904,910
Canada onroad_can	1,353,512	5,692	177,653	27,234	9,960	723	63,284
Canada othpt	1,363,501	719,783	709,218	110,273	61,060	974,147	936,907
Canada othptdust				150,439	54,777		
Canada ptfire_othna	6,282,821	104,683	134,301	685,165	580,958	60,914	1,501,988
Mexico othar	2,995,073	871,163	800,519	627,824	454,427	27,308	4,263,367
Mexico onroad_mex	5,496,594	13,807	1,336,088	108,810	83,255	36,064	574,688
Mexico othpt	1,136,851	51,548	1,215,901	374,281	265,263	2,370,238	511,462
Mexico ptfire_othna	7,136,168	120,627	347,132	1,155,991	746,107	45,222	2,260,695
Offshore cmv in Federal waters	119,908	286	530,669	13,222	12,210	16,651	31,311
Offshore cmv outside Federal waters	126,309	0	1,482,984	126,183	116,059	133,509	53,535
Offshore pt_oilgas	50,052	15	48,691	668	667	502	48,210
Non-US Total	**28,963,379**	**1,892,638**	**7,141,172**	**5,009,485**	**2,847,741**	**3,686,482**	**11,150,358**

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Appendix A: CB6 Assignment for New Species

RAMBOLL ENVIRON

September 27, 2016

MEMORANDUM

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

Summary

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

Background

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

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

Methods

CB Model Species

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

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UNC-EMAQ(4-02)-16

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Recommendation

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

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 profies 95125, 95126, and 95127
nonroad	VOC	95328	Spark-Ignition Exhaust Emissions from 2-stroke off-road engines - E10 ethanol gasoline	4.5	
nonroad	VOC	95330	Spark-Ignition Exhaust Emissions from 4-stroke off-road engines - E10 ethanol gasoline	4.5	
nonroad	VOC	95331	Diesel Exhaust Emissions from Pre-Tier 1 Off-road Engines	4.5	
nonroad	VOC	95332	Diesel Exhaust Emissions from Tier 1 Off-road Engines	4.5	
nonroad	VOC	95333	Diesel Exhaust Emissions from Tier 2 Off-road Engines	4.5	
np_oilgas	VOC	95087a	Oil and Gas - Composite - Oil Field - Oil Tank Battery Vent Gas	4.5	
np_oilgas	VOC	95109a	Oil and Gas - Composite - Oil Field - Condensate Tank Battery Vent Gas	4.5	
np_oilgas	VOC	95398	Composite Profile - Oil and Natural Gas Production - Condensate Tanks	4.5	
np_oilgas	VOC	95403	Composite Profile - Gas Wells	4.5	
np_oilgas	VOC	95417	Oil and Gas Production - Composite Profile - Untreated Natural Gas, Uinta Basin	4.5	
np_oilgas	VOC	95418	Oil and Gas Production - Composite Profile - Condensate Tank Vent Gas, Uinta Basin	4.5	
np_oilgas	VOC	95419	Oil and Gas Production - Composite Profile - Oil Tank Vent Gas, Uinta Basin	4.5	
np_oilgas	VOC	95420	Oil and Gas Production - Composite Profile - Glycol Dehydrator, Uinta Basin	4.5	

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

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

Appendix C: 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
40301001	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Fixed Roof Tanks (Varying Sizes); Gasoline RVP 13: Breathing Loss (67000 Bbl. Tank Size)
40301002	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Fixed Roof Tanks (Varying Sizes); Gasoline RVP 10: Breathing Loss (67000 Bbl. Tank Size)
40301003	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Fixed Roof Tanks (Varying Sizes); Gasoline RVP 7: Breathing Loss (67000 Bbl. Tank Size)
40301004	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Fixed Roof Tanks (Varying Sizes); Gasoline RVP 13: Breathing Loss (250000 Bbl. Tank Size)
40301006	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Fixed Roof Tanks (Varying Sizes); Gasoline RVP 7: Breathing Loss (250000 Bbl. Tank Size)
40301007	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Fixed Roof Tanks (Varying Sizes); Gasoline RVP 13: Working Loss (Tank Diameter Independent)
40301101	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Floating Roof Tanks (Varying Sizes); Gasoline RVP 13: Standing Loss (67000 Bbl. Tank Size)
40301102	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Floating Roof Tanks (Varying Sizes); Gasoline RVP 10: Standing Loss (67000 Bbl. Tank Size)
40301103	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Floating Roof Tanks (Varying Sizes); Gasoline RVP 7: Standing Loss (67000 Bbl. Tank Size)
40301105	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Floating Roof Tanks (Varying Sizes); Gasoline RVP 10: Standing Loss (250000 Bbl. Tank Size)
40301151	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Floating Roof Tanks (Varying Sizes); Gasoline: Standing Loss - Internal
40301202	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Variable Vapor Space; Gasoline RVP 10: Filling Loss
40301203	RBT	Petroleum and Solvent Evaporation; Petroleum Product Storage at Refineries; Variable Vapor Space; Gasoline RVP 7: Filling Loss
40400101	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Breathing Loss (67000 Bbl Capacity) - Fixed Roof Tank
40400102	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Breathing Loss (67000 Bbl Capacity) - Fixed Roof Tank
40400103	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Breathing Loss (67000 Bbl. Capacity) - Fixed Roof Tank
40400104	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Breathing Loss (250000 Bbl Capacity)-Fixed Roof Tank
40400105	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Breathing Loss (250000 Bbl Capacity)-Fixed Roof Tank
40400106	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Breathing Loss (250000 Bbl Capacity) - Fixed Roof Tank
40400107	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Working Loss (Diam. Independent) - Fixed Roof Tank
40400108	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Working Loss (Diameter Independent) - Fixed Roof Tank
40400109	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Working Loss (Diameter Independent) - Fixed Roof Tank
40400110	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Standing Loss (67000 Bbl Capacity)-Floating Roof Tank
40400111	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Standing Loss (67000 Bbl Capacity)-Floating Roof Tank

SCC	Type	Description
40400112	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Standing Loss (67000 Bbl Capacity)- Floating Roof Tank
40400113	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Standing Loss (250000 Bbl Cap.) - Floating Roof Tank
40400114	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Standing Loss (250000 Bbl Cap.) - Floating Roof Tank
40400115	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Standing Loss (250000 Bbl Cap.) - Floating Roof Tank
40400116	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
40400117	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
40400118	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Filling Loss (10500 Bbl Cap.) - Variable Vapor Space
40400119	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Filling Loss (10500 Bbl Cap.) - Variable Vapor Space
40400120	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Filling Loss (10500 Bbl Cap.) - Variable Vapor Space
40400130	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Specify Liquid: Standing Loss - External Floating Roof w/ Primary Seal
40400131	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Standing Loss - Ext. Floating Roof w/ Primary Seal
40400132	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Standing Loss - Ext. Floating Roof w/ Primary Seal
40400133	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Standing Loss - External Floating Roof w/ Primary Seal
40400140	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Specify Liquid: Standing Loss - Ext. Float Roof Tank w/ Secondy Seal
40400141	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Standing Loss - Ext. Floating Roof w/ Secondary Seal
40400142	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Standing Loss - Ext. Floating Roof w/ Secondary Seal
40400143	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Standing Loss - Ext. Floating Roof w/ Secondary Seal
40400148	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)
40400149	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Specify Liquid: External Floating Roof (Primary/Secondary Seal)
40400150	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Miscellaneous Losses/Leaks: Loading Racks
40400151	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Valves, Flanges, and Pumps
40400152	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Vapor Collection Losses
40400153	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Vapor Control Unit Losses
40400160	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Specify Liquid: Standing Loss - Internal Floating Roof w/ Primary Seal
40400161	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Standing Loss - Int. Floating Roof w/ Primary Seal
40400162	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Standing Loss - Int. Floating Roof w/ Primary Seal
40400163	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Standing Loss - Internal Floating Roof w/ Primary Seal
40400170	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Specify Liquid: Standing Loss - Int. Floating Roof w/ Secondary Seal

SCC	Type	Description
40400171	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 13: Standing Loss - Int. Floating Roof w/ Secondary Seal
40400172	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 10: Standing Loss - Int. Floating Roof w/ Secondary Seal
40400173	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Gasoline RVP 7: Standing Loss - Int. Floating Roof w/ Secondary Seal
40400178	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)
40400179	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; Specify Liquid: Internal Floating Roof (Primary/Secondary Seal)
40400199	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Terminals; See Comment **
40400201	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 13: Breathing Loss (67000 Bbl Capacity) - Fixed Roof Tank
40400202	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 10: Breathing Loss (67000 Bbl Capacity) - Fixed Roof Tank
40400203	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 7: Breathing Loss (67000 Bbl. Capacity) - Fixed Roof Tank
40400204	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 13: Working Loss (67000 Bbl. Capacity) - Fixed Roof Tank
40400205	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 10: Working Loss (67000 Bbl. Capacity) - Fixed Roof Tank
40400206	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 7: Working Loss (67000 Bbl. Capacity) - Fixed Roof Tank
40400207	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 13: Standing Loss (67000 Bbl Cap.) - Floating Roof Tank
40400208	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 10: Standing Loss (67000 Bbl Cap.) - Floating Roof Tank
40400210	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 13/10/7: Withdrawal Loss (67000 Bbl Cap.) - Float Rf Tnk
40400211	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 13: Filling Loss (10500 Bbl Cap.) - Variable Vapor Space
40400212	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 10: Filling Loss (10500 Bbl Cap.) - Variable Vapor Space
40400213	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 7: Filling Loss (10500 Bbl Cap.) - Variable Vapor Space
40400230	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Specify Liquid: Standing Loss - External Floating Roof w/ Primary Seal
40400231	BTP/ BPS	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
40400232	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 10: Standing Loss - Ext. Floating Roof w/ Primary Seal
40400233	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 7: Standing Loss - External Floating Roof w/ Primary Seal
40400240	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Specify Liquid: Standing Loss - Ext. Floating Roof w/ Secondary Seal
40400241	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 13: Standing Loss - Ext. Floating Roof w/ Secondary Seal
40400248	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 10/13/7: Withdrawal Loss - Ext. Float Roof (Pri/Sec Seal)
40400249	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Specify Liquid: External Floating Roof (Primary/Secondary Seal)
40400250	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Loading Racks
40400251	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Valves, Flanges, and Pumps
40400252	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Miscellaneous Losses/Leaks: Vapor Collection Losses
40400253	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Miscellaneous Losses/Leaks: Vapor Control Unit Losses
40400260	RBT	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Specify Liquid: Standing Loss - Internal Floating Roof w/ Primary Seal
40400261	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 13: Standing Loss - Int. Floating Roof w/ Primary Seal
40400262	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 10: Standing Loss - Int. Floating Roof w/ Primary Seal
40400263	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 7: Standing Loss - Internal Floating Roof w/ Primary Seal
40400270	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Specify Liquid: Standing Loss - Int. Floating Roof w/ Secondary Seal
40400271	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 13: Standing Loss - Int. Floating Roof w/ Secondary Seal
40400272	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 10: Standing Loss - Int. Floating Roof w/ Secondary Seal
40400273	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Gasoline RVP 7: Standing Loss - Int. Floating Roof w/ Secondary Seal
40400278	BTP/ BPS	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
40400279	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Specify Liquid: Internal Floating Roof (Primary/Secondary Seal)
40400401	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Petroleum Products - Underground Tanks; Gasoline RVP 13: Breathing Loss
40400402	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Petroleum Products - Underground Tanks; Gasoline RVP 13: Working Loss
40400403	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Petroleum Products - Underground Tanks; Gasoline RVP 10: Breathing Loss
40400404	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Petroleum Products - Underground Tanks; Gasoline RVP 10: Working Loss
40400405	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Petroleum Products - Underground Tanks; Gasoline RVP 7: Breathing Loss
40400406	BTP/ BPS	Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Petroleum Products - Underground Tanks; Gasoline RVP 7: Working Loss
40600101	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Splash Loading **
40600126	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Submerged Loading **
40600131	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Submerged Loading (Normal Service)
40600136	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Splash Loading (Normal Service)
40600141	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Submerged Loading (Balanced Service)
40600144	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Splash Loading (Balanced Service)
40600147	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Submerged Loading (Clean Tanks)
40600162	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Loaded with Fuel (Transit Losses)
40600163	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Gasoline: Return with Vapor (Transit Losses)
40600199	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Tank Cars and Trucks; Not Classified **
40600231	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Loading Tankers: Cleaned and Vapor Free Tanks
40600232	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Loading Tankers

SCC	Type	Description
40600233	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Loading Barges: Cleaned and Vapor Free Tanks
40600234	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Loading Tankers: Ballasted Tank
40600235	BTP/ BPS	Petroleum and Solvent Evaporation;Transportation and Marketing of Petroleum Products;Marine Vessels;Gasoline: Ocean Barges Loading - Ballasted Tank
40600236	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Loading Tankers: Uncleaned Tanks
40600237	RBT	Petroleum and Solvent Evaporation;Transportation and Marketing of Petroleum Products;Marine Vessels;Gasoline: Ocean Barges Loading - Uncleaned Tanks
40600238	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Loading Barges: Uncleaned Tanks
40600239	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Tankers: Ballasted Tank
40600240	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Loading Barges: Average Tank Condition
40600241	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Gasoline: Tanker Ballasting
40600299	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Marine Vessels; Not Classified **
40600301	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Gasoline Retail Operations - Stage I; Splash Filling
40600302	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Gasoline Retail Operations - Stage I; Submerged Filling w/o Controls
40600305	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Gasoline Retail Operations - Stage I; Unloading **
40600306	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Gasoline Retail Operations - Stage I; Balanced Submerged Filling
40600307	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Gasoline Retail Operations - Stage I; Underground Tank Breathing and Emptying
40600399	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Gasoline Retail Operations - Stage I; Not Classified **
40600401	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Filling Vehicle Gas Tanks - Stage II; Vapor Loss w/o Controls
40600501	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Pipeline Petroleum Transport - General - All Products; Pipeline Leaks
40600502	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Pipeline Petroleum Transport - General - All Products; Pipeline Venting
40600503	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Pipeline Petroleum Transport - General - All Products; Pump Station
40600504	RBT	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Pipeline Petroleum Transport - General - All Products; Pump Station Leaks
40600602	BTP/ BPS	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
40600701	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Consumer (Corporate) Fleet Refueling - Stage I; Splash Filling
40600702	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Consumer (Corporate) Fleet Refueling - Stage I; Submerged Filling w/o Controls
40600706	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Consumer (Corporate) Fleet Refueling - Stage I; Balanced Submerged Filling
40600707	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Consumer (Corporate) Fleet Refueling - Stage I; Underground Tank Breathing and Emptying
40688801	BTP/ BPS	Petroleum and Solvent Evaporation; Transportation and Marketing of Petroleum Products; Fugitive Emissions; Specify in Comments Field
2501050120	RBT	Storage and Transport; Petroleum and Petroleum Product Storage; Bulk Terminals: All Evaporative Losses; Gasoline
2501055120	BTP/ BPS	Storage and Transport; Petroleum and Petroleum Product Storage; Bulk Plants: All Evaporative Losses; Gasoline
2501060050	BTP/ BPS	Storage and Transport; Petroleum and Petroleum Product Storage; Gasoline Service Stations; Stage 1: Total
2501060051	BTP/ BPS	Storage and Transport; Petroleum and Petroleum Product Storage; Gasoline Service Stations; Stage 1: Submerged Filling
2501060052	BTP/ BPS	Storage and Transport; Petroleum and Petroleum Product Storage; Gasoline Service Stations; Stage 1: Splash Filling
2501060053	BTP/ BPS	Storage and Transport; Petroleum and Petroleum Product Storage; Gasoline Service Stations; Stage 1: Balanced Submerged Filling
2501060200	BTP/ BPS	Storage and Transport; Petroleum and Petroleum Product Storage; Gasoline Service Stations; Underground Tank: Total
2501060201	BTP/ BPS	Storage and Transport; Petroleum and Petroleum Product Storage; Gasoline Service Stations; Underground Tank: Breathing and Emptying
2501995000	BTP/ BPS	Storage and Transport; Petroleum and Petroleum Product Storage; All Storage Types: Working Loss; Total: All Products
2505000120	RBT	Storage and Transport; Petroleum and Petroleum Product Transport; All Transport Types; Gasoline
2505020120	RBT	Storage and Transport; Petroleum and Petroleum Product Transport; Marine Vessel; Gasoline
2505020121	RBT	Storage and Transport; Petroleum and Petroleum Product Transport; Marine Vessel; Gasoline - Barge
2505030120	BTP/ BPS	Storage and Transport; Petroleum and Petroleum Product Transport; Truck; Gasoline
2505040120	RBT	Storage and Transport; Petroleum and Petroleum Product Transport; Pipeline; Gasoline
2660000000	BTP/ BPS	Waste Disposal, Treatment, and Recovery; Leaking Underground Storage Tanks; Leaking Underground Storage Tanks; Total: All Storage Types