# Bayesian Space-time Downscaling Fusion Model (Downscaler) - Derived Estimates of Air Quality for 2014

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# Bayesian Space-time Downscaling Fusion Model (Downscaler) -Derived Estimates of Air Quality for 2014

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# 1.0 Introduction

This report describes estimates of daily ozone (maximum 8-hour average) and PM2.5 (24-hour average) concentrations throughout the contiguous United States during the 2014 calendar year generated by EPA's recently developed data fusion method termed the "downscaler model" (DS). Air quality monitoring data from the State and Local Air Monitoring Stations (SLAMS) and numerical output from the Community Multiscale Air Quality (CMAQ) model were both input to DS to predict concentrations at the 2010 US census tract centroids encompassed by the CMAQ modeling domain. Information on EPA's air quality monitors, CMAQ model, and downscaler model is included to provide the background and context for understanding the data output presented in this report. These estimates are intended for use by statisticians and environmental scientists interested in the daily spatial distribution of ozone and PM2.5.

DS essentially operates by calibrating CMAQ data to the observational data, and then uses the resulting relationship to predict "observed" concentrations at new spatial points in the domain. Although similar in principle to a linear regression, spatial modeling aspects have been incorporated for improving the model fit, and a Bayesian[1] approaching to fitting is used to generate an uncertainty value associated with each concentration prediction. The uncertainties that DS produces are a major distinguishing feature from earlier fusion methods previously used by EPA such as the "Hierarchical Bayesian" (HB) model (McMillan et al, 2009). The term "downscaler" refers to the fact that DS takes grid-averaged data (CMAQ) for input and produces point-based estimates, thus "scaling down" the area of data representation. Although this allows air pollution concentration estimates to be made at points where no observations exist, caution is needed when interpreting any within-gridcell spatial gradients generated by DS since they may not exist in the input datasets. The theory, development, and initial evaluation of DS can be found in the earlier papers of Berrocal, Gelfand, and Holland (2009, 2010, and 2011).

EPA's Office of Air and Radiation's (OAR) Office of Air Quality Planning and Standards (OAQPS) provides air quality monitoring data and model estimates to the Centers for Disease Control and Prevention (CDC) for use in their Environmental Public Health Tracking (EPHT) Network.CDC's EPHT Network supports linkage of air quality data with human health outcome data for use by various public health agencies throughout the U.S. The EPHT Network Program is a multidisciplinary collaboration that involves the ongoing collection, integration, analysis, interpretation, and dissemination of data from: environmental hazard monitoring activities; human exposure assessment information; and surveillance of noninfectious health conditions. As part of the National EPHT Program efforts, the CDC led the initiative to build the National EPHT Network (http:// www.cdc.gov/nceh/tracking/default.htm). The National EPHT Program, with the EPHT Network as its cornerstone, is the CDC's response to requests calling for improved understanding of how the environment affects human health. The EPHT Network is designed to provide the means to identify, access, and organize hazard, exposure, and health data from a

[1] Bayesian statistical modeling refers to methods that are based on Bayes' theorem, and model the world in terms of probabilities based on previously acquired knowledge.

variety of sources and to examine, analyze and interpret those data based on their spatial and temporal characteristics.

Since 2002, EPA has collaborated with the CDC on the development of the EPHT Network. On September 30, 2003, the Secretary of Health and Human Services (HHS) and the Administrator of EPA signed a joint Memorandum of Understanding (MOU) with the objective of advancing efforts to achieve mutual environmental public health goals[2]. HHS, acting through the CDC and the Agency for Toxic Substances and Disease Registry (ATSDR), and EPA agreed to expand their cooperative activities in support of the CDC EPHT Network and EPA's Central Data Exchange Node on the Environmental Information Exchange Network in the following areas:

- Collecting, analyzing and interpreting environmental and health data from both agencies (HHS and EPA).
- Collaborating on emerging information technology practices related to building, supporting, and operating the CDC EPHT Network and the Environmental Information Exchange Network.
- Developing and validating additional environmental public health indicators.
- Sharing reliable environmental and public health data between their respective networks in an efficient and effective manner.
- Consulting and informing each other about dissemination of results obtained through work carried out under the MOU and the associated Interagency Agreement (IAG) between EPA and CDC.

The best available statistical fusion model, air quality data, and CMAQ numerical model output were used to develop the estimates. Fusion results can vary with different inputs and fusion modeling approaches. As new and improved statistical models become available, EPA will provide updates.

Although these data have been processed on a computer system at the Environmental Protection Agency, no warranty expressed or implied is made regarding the accuracy or utility of the data on any other system or for general or scientific purposes, nor shall the act of distribution of the data constitute any such warranty. It is also strongly recommended that careful attention be paid to the contents of the metadata file associated with these data to evaluate data set limitations, restrictions or intended use. The U.S. Environmental Protection Agency shall not be held liable for improper or incorrect use of the data described and/or contained herein.

The four remaining sections and one appendix in the report are as follows:

[2] HHS and EPA agreed to extend the duration of the MOU, effective since 2002 and renewed in 2007, until June 29, 2017. The MOU is available at www.cdc.gov/nceh/tracking/partners/epa_mou_2007.htm.

- Section 2 describes the air quality data obtained from EPA's nationwide monitoring network and the importance of the monitoring data in determining health potential health risks.

- Section 3 details the emissions inventory data, how it is obtained and its role as a key input into the CMAQ air quality computer model.

- Section 4 describes the CMAQ computer model and its role in providing estimates of pollutant concentrations across the U.S. based on 12-km grid cells over the contiguous U.S.

- Section 5 explains the downscaler model used to statistically combine air quality monitoring data and air quality estimates from the CMAQ model to provide daily air quality estimates for the 2010 US census tract centroid locations within the contiguous U.S.

- The appendix provides a description of acronyms used in this report.

# 2.0 Air Quality Data

To compare health outcomes with air quality measures, it is important to understand the origins of those measures and the methods for obtaining them. This section provides a brief overview of the origins and process of air quality regulation in this country. It provides a detailed discussion of ozone ($O_3$) and particulate matter (PM). The EPHT program has focused on these two pollutants, since numerous studies have found them to be most pervasive and harmful to public health and the environment, and there are extensive monitoring and modeling data available.

## 2.1 Introduction to Air Quality Impacts in the United States

### *2.1.1 The Clean Air Act*

In 1970, the Clean Air Act (CAA) was signed into law. Under this law, EPA sets limits on how much of a pollutant can be in the air anywhere in the United States. This ensures that all Americans have the same basic health and environmental protections. The CAA has been amended several times to keep pace with new information. For more information on the CAA, go to https://www.epa.gov/clean-air-act-overview.

Under the CAA, the U.S. EPA has established standards, or limits, for six air pollutants known as the criteria air pollutants: carbon monoxide (CO), lead (Pb), nitrogen dioxide ($NO_2$), sulfur dioxide ($SO_2$), ozone ($O_3$), and particulate matter (PM). These standards, called the National Ambient Air Quality Standards (NAAQS), are designed to protect public health and the environment. The CAA established two types of air quality standards. Primary standards set limits to protect public health, including the health of "sensitive" populations such as asthmatics, children, and the elderly. Secondary standards set limits to protect public welfare, including protection against decreased visibility, damage to animals, crops, vegetation, and buildings. The CAA requires EPA to review these standards at least every five years. For more specific information on the NAAQS, go to https://www.epa.gov/criteria-air-pollutants/naaqs-table. For general information on the criteria pollutants, go to https://www.epa.gov/criteria-air-pollutants.

When these standards are not met, the area is designated as a nonattainment area. States must develop state implementation plans (SIPs) that explain the regulations and controls it will use to clean up the nonattainment areas. States with an EPA-approved SIP can request that the area be designated from nonattainment to attainment by providing three consecutive years of data showing NAAQS compliance. The state must also provide a maintenance plan to demonstrate how it will continue to comply with the NAAQS and demonstrate compliance over a 10-year period, and what corrective actions it will take should a NAAQS violation occur after designation. EPA must review and approve the NAAQS compliance data and the maintenance plan before designating the area; thus, a person may live in an area designated as nonattainment even though no NAAQS violation has been observed for quite some time. For more information on designations, go to https://www.epa.gov/ozone-designations and https://www.epa.gov/particle-pollution-designations.

### *2.1.2 Ozone*

Ozone is a colorless gas composed of three oxygen atoms. Ground level ozone is formed when pollutants released from cars, power plants, and other sources react in the presence of heat and sunlight. It is the prime ingredient of what is commonly called "smog." When inhaled, ozone can cause acute respiratory

problems, aggravate asthma, cause inflammation of lung tissue, and even temporarily decrease the lung capacity of healthy adults. Repeated exposure may permanently scar lung tissue. EPA's Integrated Science Assessments and Risk and Exposure documents are available at https://www.epa.gov/naaqs/ozone-o3-air-quality-standards. The current NAAQS for ozone (last revised in 2015) is a daily maximum 8-hour average of 0.070 parts per million [ppm] (for details, see https://www.epa.gov/ozone-pollution/setting-and-reviewing-standards-control-ozone-pollution#standards. The Clean Air Act requires EPA to review the NAAQS at least every five years and revise them as appropriate in accordance with Section 108 and Section 109 of the Act. The standards for ozone are shown in Table 2-1.

**Table 2-1. Ozone Standards**

| **Parts Per Million: Measurement – (ppm)** | **1997** | **2008** | **2015** |
|---|---|---|---|
| 4th Highest Daily Max 8-hour average | 0.08 | 0.075 | 0.070 |

### *2.1.3 Particulate Matter*

PM air pollution is a complex mixture of small and large particles of varying origin that can contain hundreds of different chemicals, including cancer-causing agents like polycyclic aromatic hydrocarbons (PAH), as well as heavy metals such as arsenic and cadmium. PM air pollution results from direct emissions of particles as well as particles formed through chemical transformations of gaseous air pollutants. The characteristics, sources, and potential health effects of particulate matter depend on its source, the season, and atmospheric conditions.

As practical convention, PM is divided by sizes into classes with differing health concerns and potential sources4. Particles less than 10 micrometers in diameter ($PM_{10}$) pose a health concern because they can be inhaled into and accumulate in the respiratory system. Particles less than 2.5 micrometers in diameter ($PM_{2.5}$) are referred to as "fine" particles. Because of their small size, fine particles can lodge deeply into the lungs. Sources of fine particles include all types of combustion (motor vehicles, power plants, wood burning, etc.) and some industrial processes. Particles with diameters between 2.5 and 10 micrometers ($PM_{10\text{-}2.5}$) are referred to as "coarse" or PMc. Sources of PMc include crushing or grinding operations and dust from paved or unpaved roads. The distribution of $PM_{10}$, $PM_{2.5}$ and PMc varies from the Eastern U.S. to arid western areas.

Particle pollution - especially fine particles - contains microscopic solids and liquid droplets that are so small that they can get deep into the lungs and cause serious health problems. Numerous scientific studies have linked particle pollution exposure to a variety of problems, including premature death in people with heart or lung disease, nonfatal heart attacks, irregular heartbeat, aggravated asthma, decreased lung function, and increased respiratory symptoms, such as irritation of airways, coughing or difficulty breathing. Additional information on the health effects of particle pollution and other technical documents related to PM standards are available at https://www.epa.gov/pm-pollution.

[4] The measure used to classify PM into sizes is the aerodynamic diameter. The measurement instruments used for PM are designed and operated to separate large particles from the smaller particles. For example, the $PM_{2.5}$ instrument only captures and thus measures particles with an aerodynamic diameter less than 2.5 micrometers. The EPA method to measure PMc is designed around taking the mathematical difference between measurements for $PM_{10}$ and $PM_{2.5}$.

The current NAAQS for $PM_{2.5}$ (last revised in 2012) includes both a 24-hour standard to protect against short-term effects, and an annual standard to protect against long-term effects. The annual average $PM_{2.5}$ concentration must not exceed 12.0 micrograms per cubic meter (ug/m$^3$) based on the annual mean concentration averaged over three years, and the 24-hr average concentration must not exceed 35 ug/m$^3$ based on the 98$^{th}$ percentile 24-hour average concentration averaged over three years. More information is available at https://www.epa.gov/pm-pollution/setting-and-reviewing-standards-control-particulate-matter-pm-pollution#standards. The standards for $PM_{2.5}$ are shown in Table 2-2.

**Table 2-2. $PM_{2.5}$ Standards**

| **Micrograms Per Cubic Meter: Measurement - (ug/m$^3$)** | **1997** | **2006** | **2012** |
|---|---|---|---|
| Annual Average | 15.0 | 15.0 | 12.0 |
| 24-Hour Average | 65 | 35 | 35 |

## 2.2 Ambient Air Quality Monitoring in the United States

### *2.2.1 Monitoring Networks*

The Clean Air Act (Section 319) requires establishment of an air quality monitoring system throughout the U.S. The monitoring stations in this network have been called the State and Local Air Monitoring Stations (SLAMS). The SLAMS network consists of approximately 4,000 monitoring sites set up and operated by state and local air pollution agencies according to specifications prescribed by EPA for monitoring methods and network design. All ambient monitoring networks selected for use in SLAMS are tested periodically to assess the quality of the SLAMS data being produced. Measurement accuracy and precision are estimated for both automated and manual methods. The individual results of these tests for each method or analyzer are reported to EPA. Then, EPA calculates quarterly integrated estimates of precision and accuracy for the SLAMS data.

The SLAMS network experienced accelerated growth throughout the 1970s. The networks were further expanded in 1999 based on the establishment of separate NAAQS for fine particles ($PM_{2.5}$) in 1997. The NAAQS for $PM_{2.5}$ were established based on their link to serious health problems ranging from increased symptoms, hospital admissions, and emergency room visits, to premature death in people with heart or lung disease. While most of the monitors in these networks are located in populated areas of the country, "background" and rural monitors are an important part of these networks. For more information on SLAMS, as well as EPA's other air monitoring networks go to https://www.epa.gov/amtic.

In 2009, approximately 43 percent of the US population was living within 10 kilometers of ozone and $PM_{2.5}$ monitoring sites. In terms of US Census Bureau tract locations, 31,341 out of 72,283 census tract centroids were within 10 kilometers of ozone monitoring sites. Highly populated Eastern US and California coasts are well covered by both ozone and $PM_{2.5}$ monitoring network (**Figure 2-1).**

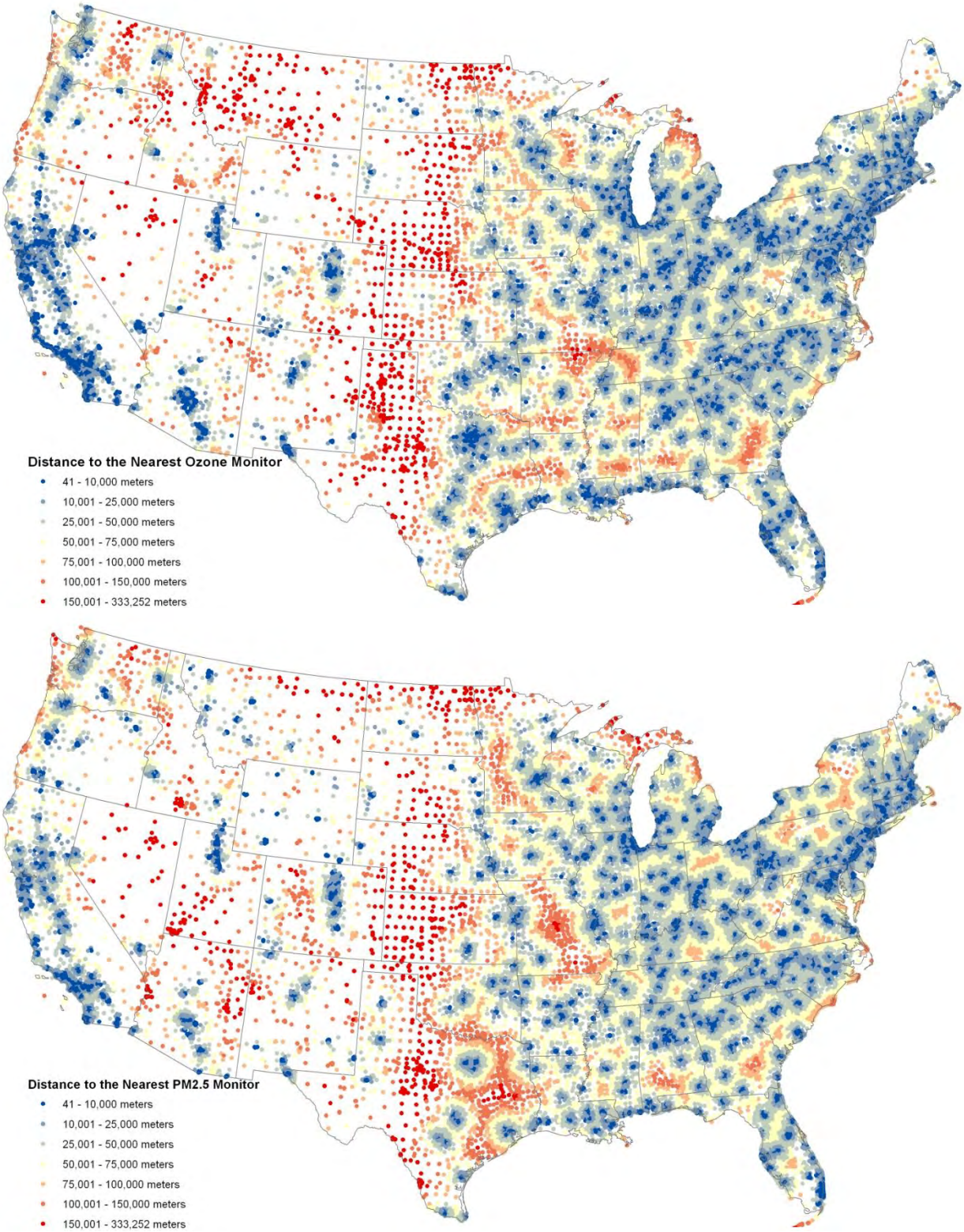


**Figure 2-1. Distances from US Census Tract centroids to the nearest monitoring site, 2009**.

In summary, state and local agencies and tribes implement a quality-assured monitoring network to measure air quality across the United States. EPA provides guidance to ensure a thorough understanding of the quality of the data produced by these networks. These monitoring data have been used to characterize the status of the nation's air quality and the trends across the U.S. (see https://www.epa.gov/air-trends).

### *2.2.2 Air Quality System Database*

EPA's Air Quality System (AQS) database contains ambient air monitoring data collected by EPA, state, local, and tribal air pollution control agencies from thousands of monitoring stations. AQS also contains meteorological data, descriptive information about each monitoring station (including its geographic location and its operator), and data quality assurance and quality control information. State and local agencies are required to submit their air quality monitoring data into AQS within 90 days following the end of the quarter in which the data were collected. This ensures timely submission of these data for use by state, local, and tribal agencies, EPA, and the public. EPA's Office of Air Quality Planning and Standards and other AQS users rely upon the data in AQS to assess air quality, assist in compliance with the NAAQS, evaluate SIPs, perform modeling for permit review analysis, and perform other air quality management functions. For more details, including how to retrieve data, go to https://www.epa.gov/aqs.

### *2.2.3 Advantages and Limitations of the Air Quality Monitoring and Reporting System*

Air quality data is required to assess public health outcomes that are affected by poor air quality. The challenge is to get surrogates for air quality on time and spatial scales that are useful for Environmental Public Health Tracking activities.

The advantage of using ambient data from EPA monitoring networks for comparing with health outcomes is that these measurements of pollution concentrations are the best characterization of the concentration of a given pollutant at a given time and location. Furthermore, the data are supported by a comprehensive quality assurance program, ensuring data of known quality. One disadvantage of using the ambient data is that it is usually out of spatial and temporal alignment with health outcomes. This spatial and temporal 'misalignment' between air quality monitoring data and health outcomes is influenced by the following key factors: the living and/or working locations (microenvironments) where a person spends their time not being co-located with an air quality monitor; time(s)/date(s) when a patient experiences a health outcome/symptom (e.g., asthma attack) not coinciding with time(s)/date(s) when an air quality monitor records ambient concentrations of a pollutant high enough to affect the symptom (e.g., asthma attack either during or shortly after a high $PM_{2.5}$ day). To compare/correlate ambient concentrations with acute health effects, daily local air quality data is needed[5]. Spatial gaps exist in the air quality monitoring network, especially in rural areas, since the air quality monitoring network is designed to focus on measurement of pollutant concentrations in high population density areas. Temporal limits also exist. Hourly ozone measurements are aggregated to daily values (the daily max 8-hour average is relevant to the ozone standard). Ozone is typically monitored during the ozone season (the warmer months, approximately April through October). However, year-long data is available in many areas and is extremely useful to evaluate whether ozone is a factor in health outcomes during the non-ozone seasons. $PM_{2.5}$ is generally measured year-round. Most Federal Reference Method (FRM) $PM_{2.5}$ monitors collect data one day in every three days, due in part to the time and costs involved in collecting and analyzing the

[5] EPA uses exposure models to evaluate the health risks and environmental effects associated with exposure. These models are limited by the availability of air quality estimates. https://www.epa.gov/technical-air-pollution-resources.

samples. However, over the past several years, continuous monitors, which can automatically collect, analyze, and report $PM_{2.5}$ measurements on an hourly basis, have been introduced. These monitors are available in most of the major metropolitan areas. Some of these continuous monitors have been determined to be equivalent to the FRM monitors for regulatory purposes and are called FEM (Federal Equivalent Methods).

### *2.2.4 Use of Air Quality Monitoring Data*

Air quality monitoring data has been used to provide the information for the following situations:

(1) Assessing effectiveness of SIPs in addressing NAAQS nonattainment areas
(2) Characterizing local, state, and national air quality status and trends
(3) Associating health and environmental damage with air quality levels/concentrations

For the EPHT effort, EPA is providing air quality data to support efforts associated with (2), and (3) above. Data supporting (3) is generated by EPA through the use of its air quality data and its downscaler model.

Most studies that associate air quality with health outcomes use air monitoring as a surrogate for exposure to the air pollutants being investigated. Many studies have used the monitoring networks operated by state and federal agencies. Some studies perform special monitoring that can better represent exposure to the air pollutants: community monitoring, near residences, in-house or work place monitoring, and personal monitoring. For the EPHT program, special monitoring is generally not supported, though it could be used on a case-by-case basis.

From proximity based exposure estimates to statistical interpolation, many approaches are developed for estimating exposures to air pollutants using ambient monitoring data (Jerrett et al., 2005). Depending upon the approach and the spatial and temporal distribution of ambient monitoring data, exposure estimates to air pollutants may vary greatly in areas further apart from monitors (Bravo et al., 2012). Factors like limited temporal coverage (i.e., $PM_{2.5}$ monitors do not operate continuously such as recording every third day or ozone monitors operate only certain part of the year) and limited spatial coverage (i. e., most monitors are located in urban areas and rural coverage is limited) hinder the ability of most of the interpolation techniques that use monitoring data alone as the input. If we look at the example of Voronoi Neighbor Averaging (VNA) (referred as the Nearest Neighbor Averaging in most literature), rural estimates would be biased towards the urban estimates. To further explain this point, assume the scenario of two cities with monitors and no monitors in the rural areas between, which is very plausible. Since exposure estimates are guaranteed to be within the range of monitors in VNA, estimates for the rural areas would be higher according to this scenario.

Air quality models may overcome some of the limitations that monitoring networks possess. Models such as the Community Multi-Scale Air Quality (CMAQ) modeling systems can estimate concentrations in reasonable temporal and spatial resolutions. However, these sophisticated air quality models are prone to systematic biases since they depend upon so many variables (i.e., metrological models and emission models) and complex chemical and physical process simulations.

Combining monitoring data with air quality models (via fusion or regression) may provide the best results

in terms of estimating ambient air concentrations in space and time. EPA's eVNA[6] is an example of an earlier approach for merging air quality monitor data with CMAQ model predictions. The downscaler model attempts to address some of the shortcomings in these earlier attempts to statistically combine monitor and model predicted data, see published paper referenced in section 1 for more information about the downscaler model. As discussed in the next section, there are two methods used in EPHT to provide estimates of ambient concentrations of air pollutants: air quality monitoring data and the downscaler model estimate, which is a statistical 'combination' of air quality monitor data and photochemical air quality model predictions (e.g., CMAQ).

## 2.3 Air Quality Indicators Developed for the EPHT Network

Air quality indicators have been developed for use in the Environmental Public Health Tracking Network by CDC using the ozone and $PM_{2.5}$ data from EPA. The approach used divides "indicators" into two categories. First, basic air quality measures were developed to compare air quality levels over space and time within a public health context (e.g., using the NAAQS as a benchmark). Next, indicators were developed that mathematically link air quality data to public health tracking data (e.g., daily $PM_{2.5}$ levels and hospitalization data for acute myocardial infarction). Table 2-3 and Table 2-4 describe the issues impacting calculation of basic air quality indicators.

**Table 2-2. Public Health Surveillance Goals and Current Status**

| Goal | Status |
|---|---|
| Air data sets and metadata required for air quality indicators are available to EPHT state Grantees. | AQS data are available through state agencies and EPA's Air Quality System (AQS). EPA and CDC developed an interagency agreement, where EPA provides air quality data along with statistically combined AQS and Community Multiscale Air Quality (CMAQ) Model data, associated metadata, and technical reports that are delivered to CDC. |
| Estimate the linkage or association of $PM_{2.5}$ and ozone on health to: Identify populations that may have higher risk of adverse health effects due to $PM_{2.5}$ and ozone,<br><br>Generate hypothesis for further research, and<br><br>Provide information to support prevention and pollution control strategies. | Regular discussions have been held on health-air linked indicators and CDC/HFI/EPA convened a workshop January 2008. CDC has collaborated on a health impact assessment (HIA) with Emory University, EPA, and state grantees that can be used to facilitate greater understanding of these linkages. |
| Produce and disseminate basic indicators and other findings in electronic and print formats to provide the public, environmental health professionals, and policymakers, with current and easy-to-use information about air pollution and the impact on public health. | Templates and "how to" guides for $PM_{2.5}$ and ozone have been developed for routine indicators. Calculation techniques and presentations for the indicators have been developed. |

[6] eVNA is described in the "Regulatory Impact Analysis for the Final Clean Air Interstate Rule", EPA-452/R-05-002, March 2005, Appendix F.

**Table 2-3. Basic Air Quality Indicators used in EPHT, derived from the EPA data delivered to CDC**

| Ozone (daily 8-hr period with maximum concentration—ppm—by Federal Reference Method (FRM)) |
|---|
| • Number of days with maximum ozone concentration over the NAAQS (or other relevant benchmarks (by county and MSA)<br>• Number of person-days with maximum 8-hr average ozone concentration over the NAAQS & other relevant benchmarks (by county and MSA) |
| $PM_{2.5}$ (daily 24-hr integrated samples –ug/m$^3$-by FRM) |
| • Average ambient concentrations of particulate matter (< 2.5 microns in diameter) and compared to annual $PM_{2.5}$ NAAQS (by state).<br>• % population exceeding annual $PM_{2.5}$ NAAQS (by state).<br>• % of days with $PM_{2.5}$ concentration over the daily NAAQS (or other relevant benchmarks (by county and MSA)<br>• Number of person-days with $PM_{2.5}$ concentration over the daily NAAQS & other relevant benchmarks (by county and MSA) |

### *2.3.1 Rationale for the Air Quality Indicators*

The CDC EPHT Network is initially focusing on ozone and $PM_{2.5}$. These air quality indicators are based mainly around the NAAQS health findings and program-based measures (measurement, data and analysis methodologies). The indicators will allow comparisons across space and time for EPHT actions. They are in the context of health-based benchmarks. By bringing population into the measures, they roughly distinguish between potential exposures (at broad scale).

### *2.3.2 Air Quality Data Sources*

The air quality data will be available in the US EPA Air Quality System (AQS) database based on the state/federal air program's data collection and processing. The AQS database contains ambient air pollution data collected by EPA, state, local, and tribal air pollution control agencies from thousands of monitoring stations (SLAMS).

### *2.3.3 Use of Air Quality Indicators for Public Health Practice*

The basic indicators will be used to inform policymakers and the public regarding the degree of hazard within a state and across states (national). For example, the number of days per year that ozone is above the NAAQS can be used to communicate to sensitive populations (such as asthmatics) the number of days that they may be exposed to unhealthy levels of ozone. This is the same level used in the Air Quality Alerts that inform these sensitive populations when and how to reduce their exposure. These indicators, however, are not a surrogate measure of exposure and therefore will not be linked with health data.

# 3.0 Emissions Data

## 3.1 Introduction to Emissions Data Development

The U.S. Environmental Protection Agency (EPA) developed an air quality modeling platform based primarily on the 2014 National Emissions Inventory (NEI), Version 1 to process year 2014 emission data for this project. This section provides a summary of the emissions inventory and emissions modeling techniques applied to Criteria Air Pollutants (CAPs) and the following select Hazardous Air Pollutants (HAPs) included in the modeling platform: chlorine (Cl), hydrogen chloride (HCl), benzene, acetaldehyde, formaldehyde, napthalene and methanol. This section also describes the approach and data used to produce emissions inputs to the air quality model. The air quality modeling, meteorological inputs and boundary conditions are described in a separate section.

The Community Multiscale Air Quality (CMAQ) model (http://www.epa.gov/AMD/CMAQ/) was used to model ozone ($O_3$) and particulate matter (PM) for this project. CMAQ requires hourly and gridded emissions of the following inventory pollutants: carbon monoxide (CO), nitrogen oxides ($NO_X$), volatile organic compounds (VOC), sulfur dioxide ($SO_2$), ammonia ($NH_3$), particulate matter less than or equal to 10 microns ($PM_{10}$), and individual component species for particulate matter less than or equal to 2.5 microns ($PM_{2.5}$). In addition, the Carbon bond version 6 (CB6) with chlorine chemistry used here within CMAQ allows for explicit treatment of the VOC HAPs naphthalene, benzene, acetaldehyde, formaldehyde and methanol (NBAFM) and includes anthropogenic HAP emissions of HCl and Cl.

The effort to create the 2014 emission inputs for this study included development of emission inventories for input to a 2014 modeling case, along with application of emissions modeling tools to convert the inventories into the format and resolution needed by CMAQ. Year-specific fire and continuous emission monitoring (CEM) data for electric generating units (EGUs) were used. The primary emissions modeling tool used to create the CMAQ model-ready emissions was the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system. SMOKE version 4.5 was used to create CMAQ-ready emissions files for a 12-km national grid. Additional information about SMOKE is available from http://cmascenter.org/smoke.

This chapter contains two additional sections. Section 3.2 describes the inventories input to SMOKE and the ancillary files used along with the emission inventories. Section 3.3 describes the emissions modeling performed to convert the inventories into the format and resolution needed by CMAQ.

## 3.2 Emission Inventories and Approaches

This section describes the emissions inventories created for input to SMOKE. The 2014 NEI, version 1 with some updates is the primary basis for the inputs to SMOKE. The NEI includes five main data categories: a) nonpoint (formerly called "stationary area") sources; b) point sources; c) nonroad mobile sources; d) onroad mobile sources; and e) fires. For CAPs, the NEI data are largely compiled from data submitted by state, local and tribal (S/L/T) agencies. HAP emissions data are often augmented by EPA when they are not voluntarily submitted to the NEI by S/L/T agencies. The NEI was compiled using the

Emissions Inventory System (EIS). EIS includes hundreds of automated QA checks to improve data quality, and it also supports release point (stack) coordinates separately from facility coordinates. EPA collaboration with S/L/T agencies helped prevent duplication between point and nonpoint source categories such as industrial boilers. The 2014 NEI Technical Support Document is available at https://www.epa.gov/air-emissions-inventories/2014-national-emissions-inventory-nei-technical-support-document-tsd (EPA, 2016).

Point source data for the year 2014 as submitted to EIS were used for this study. EPA used the SMARTFIRE2 system to develop 2014 fire emissions. SMARTFIRE2 categorizes all fires as either prescribed burning or wildfire categories, and includes improved emission factor estimates for prescribed burning. Onroad and nonroad mobile source emissions for year 2014 were developed using MOVES2014a. Canadian emissions reflect year 2013 and Mexican emissions reflect year 2014.

The methods used to process emissions for this study are similar to those documented for EPA's Version 7, 2014 Emissions Modeling Platform that was also used for the preliminary version of the 2014 National Air Toxics Assessment (NATA), with the exception that many fewer HAPs are included in this platform. A technical support document (TSD) for the 2014v7 platform is available here https://www.epa.gov/air-emissions-modeling/2014-version-70-technical-support-document-tsd (EPA, 2017a) and includes additional details regarding the data preparation and emissions modeling with the exception of the HAP speciation.

The emissions modeling process, performed using SMOKE v4.5, apportions the emissions inventories into the grid cells used by CMAQ and temporalizes the emissions into hourly values. In addition, the pollutants in the inventories (e.g., NOx, PM and VOC) are split into the chemical species needed by CMAQ. For the purposes of preparing the CMAQ- ready emissions, the NEI emissions inventories by data category are split into emissions modeling "platform" sectors; and emissions from sources other than the NEI are added, such as the Canadian, Mexican, and offshore inventories. Emissions sectors within the emissions modeling platform are separated out from each other when the emissions for that sector are run through all of the SMOKE programs, except the final merge, independently from emissions in the other sectors. The final merge program called Mrggrid combines the sector-specific gridded, speciated and temporalized emissions to create the final CMAQ-ready emissions inputs. Biogenic emissions are computed and used by CMAQ as it runs.

Table 3-1 presents the sectors in the emissions modeling platform used to develop the year 2014 emissions for this project. The sector abbreviations are provided in italics; these abbreviations are used in the SMOKE modeling scripts, the inventory file names, and throughout the remainder of this section. Annual 2014 emission summaries for the U.S. anthropogenic sectors are shown in Table 3-2 (i.e., biogenic emissions are excluded). Table 3-3 provides a summary of emissions for the anthropogenic sectors containing Canadian, Mexican and offshore sources. State total emissions for each sector are provided in Appendix B, a workbook entitled "Appendix_B_2014_emissions_totals_by_sector.xlsx".

**Table 3-1. Platform Sectors Used in the Emissions Modeling Process**

| 2014 Platform Sector *(Abbrev)* | NEI Category | Description and resolution of the data input to SMOKE |
|---|---|---|
| EGUs (*ptegu)* | Point | 2014 point source EGUs. Replaced with hourly 2014 Continuous Emissions Monitoring System (CEMS) values for NOX and SO2, where the units are matched to the NEI. Emissions for all sources not matched to CEMS data come from 2014NEIv1. Annual resolution for sources not matched to CEMS data, hourly for CEMS sources. |
| Point source oil and gas (*pt_oilgas)* | Point | 2014NEIv1 point sources that include oil and gas production emissions processes based on facilities with the following NAICS: 211* (Oil and Gas Extraction), 213111 (Drilling Oil and Gas Wells) 213112 (Support Activities for Oil and Gas Operations), 4861* (Pipeline Transportation of Crude Oil), 4862* (Pipeline Transportation of Natural Gas). Includes U.S. offshore oil production. Annual resolution. |
| Remaining non-EGU point (*ptnonipm*) | Point | All 2014NEIv1 point source records not matched to the ptegu or pt_oilgas sectors. Includes all aircraft and airport ground support emissions and some rail yard emissions. Annual resolution. |
| Point source fire (*ptfire*) | Fires | Point source day-specific wildfires and prescribed fires for 2014 computed using SMARTFIRE 2. Fires over 20,000 acres on a single day allocated to overlapping grid cells. |
| Point Source agricultural fires (ptagfire) | Nonpoint | Agricultural fire sources that were developed by EPA as point and day-specific emissions; they were put into the nonpoint data category of the NEI, but in the platform, they are treated as point sources. |
| Agricultural (*ag*) | Nonpoint | Ammonia emissions from 2014NEIv2 nonpoint livestock and 2014NEIv1 fertilizer application; county and annual resolution. |
| Area fugitive dust (*afdust_adj*) | Nonpoint | $PM_{10}$ and $PM_{2.5}$ fugitive dust sources from the 2014NEIv1 nonpoint inventory; including building construction, road construction, agricultural dust, and road dust. The emissions modeling adjustment applies a transport fraction and a meteorology-based (precipitation and snow/ice cover) zero-out. County and annual resolution. |
| Biogenic (*beis*) | Nonpoint | Biogenic emissions were left out of the CMAQ-ready merged emissions, in favor of inline biogenics produced during the CMAQ model run itself. |
| C1 and C2 commercial marine (*cmv_c1c2*) | Nonpoint | 2014NEIv1 Category 1 (C1) and Category 2 (C2), commercial marine vessel (CMV) emissions. County and annual resolution. |
| C3 commercial marine (*cmv_c3*) | Nonpoint | Within state waters, 2014NEIv1 Category 3 commercial marine vessel (CMV) emissions. Outside of state waters emissions are based on the Emissions Control Area (ECA) inventory. Point (to allow for plume rise) and annual resolution. |
| Remaining nonpoint (*nonpt*) | Nonpoint | 2014NEIv1 nonpoint sources not included in other platform sectors with adjustments to remove chromium from fugitive |

| 2014 Platform Sector *(Abbrev)* | NEI Category | Description and resolution of the data input to SMOKE |
|---|---|---|
| | | dust categories (paved and unpaved roads, construction and crops and livestock). County and annual resolution. |
| Nonpoint source oil and gas (*np_oilgas)* | Nonpoint | 2014NEIv1 nonpoint sources from oil and gas-related processes with specific adjustment in four unitah basin counties in Utah to correct EPA augmented benzene, toluene, ethylbenzene and xylenes. County and annual resolution. |
| Locomotive (*rail*) | Nonpoint | Rail locomotives emissions from the 2014NEIv1. County and annual resolution. |
| Residential Wood Combustion (*rwc*) | Nonpoint | 2014NEIv1 nonpoint sources with residential wood combustion (RWC) processes. County and annual resolution. |
| Nonroad (*nonroad*) | Nonroad | 2014NEIv1 nonroad equipment emissions developed with the MOVES2014a using NONROAD2008 version NR08a and new HAP emission factors than had been used in the 2011NEI. MOVES was used for all states except California, which submitted their own emissions for the 2014NEIv1. County and monthly resolution. |
| Onroad (*onroad*) | Onroad | 2014 onroad mobile source gasoline and diesel vehicles from parking lots and moving vehicles. Includes the following modes: exhaust, extended idle, auxiliary power units, evaporative, permeation, refueling, and brake and tire wear. For all states except California, developed using winter and summer MOVES emission factors tables produced by MOVES2014a. |
| Onroad California (*onroad_ca_adj*) | Onroad | 2014 California-provided CAP and metal HAP onroad mobile source gasoline and diesel vehicles from parking lots and moving vehicles based on Emission Factor (EMFAC), gridded and temporalized using MOVES2014a. Volatile organic compound (VOC) HAP emissions derived from California-provided VOC emissions and MOVES-based speciation. |
| Onroad Canada (*onroad_can*) | Non-US | Monthly year 2013 Canada (province resolution) onroad mobile inventory. |
| Onroad Mexico (*onroad_mex*) | Non-US | Monthly year 2014 Mexico (municipio resolution) onroad mobile inventory. |
| Other area fugitive dust sources | Non-US | Area fugitive dust sources from Canada 2013 inventory with transport fraction and snow/ice adjustments based on 2014 meteorological data. Annual and province resolution. |

| 2014 Platform Sector *(Abbrev)* | NEI Category | Description and resolution of the data input to SMOKE |
|---|---|---|
| Other nonpoint and nonroad (*othar*) | Non-US | Year 2013 Canada (province resolution) and projected year 2014 Mexico (municipio resolution) nonpoint and nonroad mobile inventories, annual resolution. |
| Other point sources not from the NEI (*othpt*) | Non-US | Point sources from Canada's 2013 inventory and Mexico point sources projected to 2014. Annual resolution. |
| Point fires in Mexico and Canada (ptfire_mxca) | Non-US | Point source day-specific wildfires and prescribed fires for 2014 provided by Environment Canada with data for missing months and for Mexico filled in using fires from the Fire INventory (FINN) from National Center for Atmospheric Research (NCAR) fires (NCAR, 2016 and Wiedinmyer, C., 2011). |

**Table 32. 2014 Continental United States Emissions by Sector (tons/yr in 48 states + D.C.)**

| Sector | CO | $NH_3$ | $NO_x$ | $PM_{10}$ | $PM_{2.5}$ | $SO_2$ | VOC |
|---|---|---|---|---|---|---|---|
| **afdust_adj** | | | | 6,991,664 | 975,147 | | |
| **ag** | | 2,867,904 | | | | | |
| **cmv_c1c2** | 44,808 | 109 | 227,954 | 5,978 | 5,737 | 3,387 | 4,488 |
| **cmv_c3** | 11,300 | 28 | 112,333 | 4,221 | 3,809 | 38,721 | 5,248 |
| **nonpt** | 2,894,351 | 114,049 | 794,416 | 712,611 | 569,249 | 300,871 | 3,571,099 |
| **np_oilgas** | 820,021 | 15 | 793,601 | 20,628 | 20,196 | 37,794 | 3,104,473 |
| **nonroad** | 12,425,532 | 2,244 | 1,392,082 | 140,863 | 133,362 | 3,163 | 1,630,321 |
| **onroad** | 21,548,865 | 103,333 | 4,622,945 | 307,113 | 157,997 | 28,324 | 2,170,529 |
| **ptagfire** | 426,253 | 55,639 | 12,897 | 69,528 | 49,398 | 3,870 | 25,816 |
| **ptfire** | 16,949,926 | 273,912 | 246,873 | 1,746,224 | 1,481,934 | 130,085 | 3,921,240 |
| **ptegu** | 735,826 | 25,933 | 1,758,567 | 236,027 | 183,029 | 3,241,498 | 35,523 |
| **ptnonipm** | 2,055,540 | 64,809 | 1,193,886 | 525,313 | 292,816 | 880,822 | 828,083 |
| **pt_oilgas** | 190,142 | 333 | 398,535 | 11,652 | 11,165 | 43,576 | 132,875 |
| **rail** | 119,252 | 364 | 779,801 | 25,094 | 23,166 | 6,986 | 39,857 |
| **rwc** | 2,156,051 | 16,221 | 32,174 | 333,219 | 332,700 | 8,087 | 351,696 |
| **Continental U.S.** | **60,377,867** | **3,524,893** | **12,366,065** | **11,130,134** | **4,239,702** | **4,727,182** | **15,821,249** |

**Table 33. 2014 Non-US Emissions by Sector within Modeling Domain (tons/yr for Canada, Mexico, Offshore)**

| Sector | CO | $NH_3$ | $NO_X$ | $PM_{10}$ | $PM_{2.5}$ | $SO_2$ | VOC |
|---|---|---|---|---|---|---|---|
| Canada othafdust | | | | 1,725,731 | 338,480 | | |
| Canada othar | 2,809,336 | 496,889 | 615,888 | 414,236 | 228,545 | 62,379 | 1,101,710 |
| Canada onroad_can | 2,105,867 | 8,446 | 474,813 | 28,204 | 21,474 | 1,593 | 191,505 |
| Canada othpt | 1,102,908 | 17,323 | 646,981 | 91,095 | 47,323 | 999,891 | 782,440 |
| Canada ptfire_mxca | 6,701,372 | 4,574 | 150,552 | 730,230 | 618,866 | 66,034 | 1,629,916 |
| **Canada Subtotal** | **12,719,483** | **527,233** | **1,888,235** | **2,989,497** | **1,254,688** | **1,129,897** | **3,705,570** |
| Mexico othar | 232,017 | 206,491 | 212,636 | 114,414 | 53,378 | 7,628 | 503,968 |
| Mexico onroad_mex | 1,823,639 | 2,660 | 432,368 | 14,716 | 10,649 | 5,849 | 158,524 |
| Mexico othpt | 188,253 | 4,669 | 465,960 | 72,872 | 57,479 | 543,591 | 66,392 |
| Mexico ptfire_mxca | 251,658 | 4,875 | 11,048 | 29,482 | 24,900 | 1,813 | 86,215 |
| **Mexico Subtotal** | **2,495,567** | **218,695** | **1,122,012** | **231,483** | **146,406** | **558,882** | **815,100** |
| Offshore to EEZ | 109,269 | 183 | 873,194 | 26,989 | 25,142 | 148,445 | 27,864 |
| Non-US SECA C3 | 32,807 | 0 | 386,133 | 32,865 | 30,234 | 243,088 | 13,904 |
| **2014 Total non-U.S.** | **15,357,126** | **746,111** | **4,269,573** | **3,280,833** | **1,456,471** | **2,080,312** | **4,562,438** |

### *3.2.1 Point Sources (ptegu, pt_oilgas and ptnonipm)*

Point sources are sources of emissions for which specific geographic coordinates (e.g., latitude/longitude) are specified, as in the case of an individual facility. A facility may have multiple emission release points that may be characterized as units such as boilers, reactors, spray booths, kilns, etc. A unit may have multiple processes (e.g., a boiler that sometimes burns residual oil and sometimes burns natural gas). With a couple of minor exceptions, this section describes only NEI point sources within the contiguous U.S. The offshore oil platform (pt_oilgas sector) and category 3 CMV emissions (cmv_c3 sector) are processed by SMOKE as point source inventories and are discussed later in this section. A complete NEI is developed every three years, with 2014 being the most recently finished complete NEI. A comprehensive description about the development of the 2014NEIv1 is available in the 2014NEIv1 TSD (EPA, 2016a).

In preparation for modeling, the complete set of point sources in the NEI was exported from EIS into the Flat File 2010 (FF10) format that is compatible with SMOKE (see https://www.cmascenter.org/smoke/documentation/4.0/html/ch08s02s08.html) and was then split into several sectors for modeling. After moving offshore oil platforms into the othpt sector, and dropping sources without specific locations (i.e., the FIPS code ends in 777), initial versions of inventories for the other three point source sectors were created from the remaining 2014 point sources. The point sectors are: EGUs (ptegu), point source oil and gas extraction-related sources (pt_oilgas) and the remaining non-EGUs (ptnonipm). The EGU emissions are split out from the other sources to facilitate the use of distinct SMOKE temporal processing and future-year projection techniques. The oil and gas sector emissions (pt_oilgas) were processed separately for summary tracking purposes and distinct future-year projection techniques from the remaining non-EGU emissions (ptnonipm).

The inventory pollutants processed through SMOKE for both the ptipm and ptnonipm sectors were: CO, NOX, VOC, SO2, NH3, PM10, and PM2.5 and the following HAPs: HCl (pollutant code = 7647010), and Cl (code = 7782505). NBAFM pollutants from the point sectors were not utilized because VOC was speciated without the use (i.e., integration) of VOC HAP pollutants from the inventory.

The ptnonipm and pt_oilgas sector emissions were provided to SMOKE as annual emissions. For sources in the ptegu sector that could be matched to 2014 CEMS data, hourly CEMS $NO_X$ and $SO_2$ emissions for 2014 from EPA's Acid Rain Program were used rather than NEI emissions. For all other pollutants (e.g., VOC, $PM_{2.5}$, HCl), annual emissions were used as-is from the NEI, but were allocated to hourly values using heat input from the CEMS data. For the unmatched units in the ptegu sector, annual emissions were allocated to daily values using IPM region- and pollutant-specific profiles, and similarly, region- and pollutant-specific diurnal profiles were applied to create hourly emissions.

The non-EGU stationary point source (ptnonipm) emissions were input to SMOKE as annual emissions. The full description of how the NEI emissions were developed is provided in the NEI documentation, but a brief summary of their development follows:

a. CAP and HAP data were provided by States, locals and tribes under the Air Emissions Reporting Rule (AERR)
b. EPA corrected known issues and filled PM data gaps.
c. EPA added HAP data from the Toxic Release Inventory (TRI) where corresponding data was not

already provided by states/locals.

d. EPA provided data for airports and rail yards.
e. Off-shore platform data were added from the Bureau of Ocean Energy Management (BOEM).

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

- The tribal data, which do not use state/county Federal Information Processing Standards (FIPS) codes in the NEI, but rather use the tribal code, were assigned a state/county FIPS code of 88XXX, where XXX is the 3-digit tribal code in the NEI. This change was made because SMOKE requires all sources to have a state/county FIPS code.
- Sources that did not have specific counties assigned (i.e., the county code ends in 777) were not included in the modeling because it was only possible to know the state in which the sources resided, but no more specific details related to the location of the sources were available.
- Stack parameters for point sources missing this information were filled in prior to modeling in SMOKE.

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

#### *3.2.1.1 EGU sector (ptegu)*

The ptegu sector contains emissions from EGUs in the 2014 point source inventory that could be matched to units found in the National Electric Energy Database System (NEEDS) v5.16 that is used by the Integrated Planning Model (IPM) to develop future year EGU emissions. It was necessary to put these EGUs into a separate sector in the platform because EGUs use different temporal profiles than other sources in the point sector and it is useful to segregate these emissions from the rest of the point sources to facilitate summaries of the data. Sources not matched to units found in NEEDS are placed into the pt_oilgas or ptnonipm sectors. For studies with future year cases, the sources in the ptegu sector are fully replaced with the emissions output from IPM. It is therefore important that the matching between the NEI and NEEDS database be as complete as possible because there can be double-counting of emissions in future year modeling scenarios if emissions for units are projected by IPM are not properly matched to the units in the point source inventory.

Some units in the ptegu sector are matched to CEMS data via ORIS facility codes and boiler ID. For these units, SMOKE replaces the emissions of NOX and SO2 with the CEMS emissions, thereby ignoring the annual values specified in the point source inventory. For other pollutants, the hourly CEMS heat input data are used to allocate the ptegu inventory annual emissions to hourly values. All stack parameters, stack locations, and SCC codes for these sources come from the point source inventory. Because these attributes are obtained from the inventory, the chemical speciation of VOC and PM2.5 for the sources is selected based on the SCC or in some cases, based on unit-specific data. If CEMS data exists for a unit, but the unit is not matched to the inventory, the CEMS data for that unit is not used in the modeling platform. However, if the source exists in the inventory and is not matched to a CEMS unit, the emissions from that source would be modeled using the annual emission value in the inventory and would be allocated to daily values using region-, fuel- and pollutant-specific average profiles. EIS stores many matches from EIS units to the ORIS facility codes and boiler IDs used to reference the CEMS data. Some additional matches were made at the release point level in the emissions modeling platform.

For sources not matched to CEMS data, daily emissions were computed from the NEI annual emissions using average CEMS data profiles specific to fuel type, pollutant (i.e., $NO_x$, $SO_2$, and other), and IPM region. Note that pollutants other than $NO_x$, $SO_2$ are allocated based on heat input. To allocate emissions to each hour of the day, diurnal profiles were created using average CEMS data for heat input specific to fuel type and IPM region. Sources identified as municipal waste combustors and co-generation units were temporally allocated using the same emissions for each hour of the year because these sources are assumed to operate at the same level continuously.

#### *3.2.1.2 Point Oil and Gas Sector (pt_oilgas)*

The pt_oilgas sector was separated from the ptnonipm sector by selecting sources with specific North American Industry Classification System (NAICS) codes shown in Table 3-4. The emissions and other source characteristics in the pt_oilgas sector are submitted by states, while EPA developed a dataset of nonpoint oil and gas emissions for each county in the U.S. with oil and gas activity that was available for states to use. Nonpoint oil and gas emissions can be found in the np_oilgas sector. More information on the development of the 2014 oil and gas emissions can be found in Section 4.16 of the 2014NEIv1 TSD. The pt_oilgas sector includes emissions from offshore oil platforms.

**Table 3-4.** Point source oil and gas sector NAICS Codes

| NAICS | NAICS description |
|---|---|
| 2111 | Oil and Gas Extraction |
| 4862 | Pipeline Transportation of Natural Gas |
| 21111 | Oil and Gas Extraction |
| 48611 | Pipeline Transportation of Crude Oil |
| 48621 | Pipeline Transportation of Natural Gas |
| 211111 | Crude Petroleum and Natural Gas Extraction |
| 211112 | Natural Gas Liquid Extraction |
| 213111 | Drilling Oil and Gas Wells |
| 213112 | Support Activities for Oil and Gas Operations |
| 486110 | Pipeline Transportation of Crude Oil |
| 486210 | Pipeline Transportation of Natural Gas |

#### *3.2.1.3 Non-IPM Sector (ptnonipm)*

Except for some minor exceptions, the non-IPM (ptnonipm) sector contains the point sources that are not in the ptegu or pt_oilgas sectors. For the most part, the ptnonipm sector reflects the non-EGU sources of the NEI point inventory; however, it is likely that some low-emitting EGUs not matched to the NEEDS database or to CEMS data are in the ptnonipm sector.

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

### *3.2.2 Day-Specific Point Source Fires (ptfire)*

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

The point source day-specific emission estimates for 2014 fires were developed using SMARTFIRE 2 (Sullivan, et al., 2008), which uses the National Oceanic and Atmospheric Administration's (NOAA's) Hazard Mapping System (HMS) fire location information and for 2014 also uses state/local/tribal data as input. Additional inputs include the CONSUMEv3.0 software application (Joint Fire Science Program, 2009) and the Fuel Characteristic Classification System (FCCS) fuel-loading database to estimate fire emissions from wildfires and prescribed burns on a daily basis. The method involves the reconciliation of ICS-209 reports (Incident Status Summary Reports) and GeoMAC Shapefiles with satellite-based fire detections to determine spatial and temporal information about the fires. A functional diagram of the SMARTFIRE 2 process of reconciling fires with ICS-209 reports is available in the documentation (Raffuse, et al., 2007). Once the fire reconciliation process is completed, the emissions are calculated using the U.S. Forest Service's CONSUMEv3.0 fuel consumption model and the FCCS fuel-loading database in the BlueSky Framework (Ottmar, et. al., 2007). More information is available in the 2014NEIv1 TSD.

A difference between the fires for this study and those in the NEI is that the proportion of emissions allocated to flaming versus smoldering SCCs were adjusted. Flaming fractions were calculated for each fire based on the flaming and smoldering consumption divided by the total consumption. Smoldering fractions were calculated by dividing the residual consumption by the total consumption. The fractions were then applied to the fire emissions in the 2014NEIv1 to obtained revised emissions for the flaming and smoldering SCCs. The total emissions by state were unchanged, but they were reapportioned to the flaming and smoldering SCCs to facilitate a more realistic plume rise for fires. Washington state emissions were adjusted according to emissions supplied by the state. Monthly factors of state data to NEI data by county, SCC, and pollutant were calculated then applied to the existing daily and annual emissions data in the FF10 for Washington state only.

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

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

### *3.2.3 Nonpoint Sources (afdust, ag, nonpt, np_oilgas, rwc)*

Several modeling platform sectors were created from the 2014NEIv1 nonpoint inventory. This section describes the *stationary* nonpoint sources. Locomotives, C1 and C2 CMV, and C3 CMV are also included the 2014NEIv1 nonpoint data category, but are mobile sources and are described in a later section. The 2014NEIv1 TSD includes documentation for the nonpoint data.

The nonpoint tribal-submitted emissions are dropped during spatial processing with SMOKE due to the configuration of the spatial surrogates, which are available by county, but not at the tribal level. In addition, possible double-counting with county-level emissions is prevented. These omissions are not expected to have an impact on the results of the air quality modeling at the 12-km scales used for this platform.

In the rest of this section, each of the platform sectors into which the 2014 nonpoint NEI was divided is described, along with any data that were updated or replaced with non-NEI data.

#### *3.2.3.1 Area Fugitive Dust Sector (afdust)*

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

The afdust sector is separated from other nonpoint sectors to allow for the application of a "transport fraction," and meteorological/precipitation reductions. These adjustments are applied with a script that applies land use-based gridded transport fractions followed by another script that zeroes out emissions for days on which at least 0.01 inches of precipitation occurs or there is snow cover on the ground. The land use data used to reduce the NEI emissions determines the amount of emissions that are subject to transport. This methodology is discussed in (Pouliot, et al., 2010), https://www3.epa.gov/ttn/chief/conference/ei19/session9/pouliot_pres.pdf, and in "Fugitive Dust Modeling for the 2008 Emissions Modeling Platform" (Adelman, 2012). Both the transport fraction and meteorological adjustments are based on the gridded resolution of the platform (e.g., 12km grid cells); therefore, different emissions will result if the process were applied to different grid resolutions. A limitation of the transport fraction approach is the lack of monthly variability that would be expected with seasonal changes in vegetative cover. While wind speed and direction are not accounted for in the emissions processing, the hourly variability due to soil moisture, snow cover and precipitation is accounted for in the subsequent meteorological adjustment.

Where states submitted afdust data, it was assumed that the state-submitted data were not met-adjusted and therefore the meteorological adjustments were applied. Thus, if states submitted data that were met-adjusted, these sources would have been adjusted for meteorology twice. Even with that possibility, air quality modeling shows that, in general, dust is frequently overestimated in the air quality modeling results.

### *3.2.3.2 Agricultural Ammonia Sector (ag)*

The agricultural $NH_3$ (ag) sector includes livestock emissions from the 2014NEIv2 nonpoint inventory and agricultural fertilizer application emissions from the 2014NEIv1 nonpoint inventory. The livestock and fertilizer emissions in this sector are based only on the SCCs starting with 2805 and 2801. The livestock SCCs are related to beef and dairy cattle, poultry production and waste, swine production, waste from horses and ponies, and production and waste for sheep, lambs, and goats. The fertilizer SCCs consist of 15 specific types of ammonia-based fertilizer and one for miscellaneous fertilizers. The "ag" sector includes all of the $NH_3$ emissions from fertilizer from the NEI. However, the "ag" sector does not include all of the livestock $NH_3$ emissions, as there is a very small amount of $NH_3$ emissions from livestock in the ptnonipm inventory (as point sources) in California (883 tons; less than 0.5 percent of state total) and Wisconsin (356 tons; about 1 percent of state total).

The agricultural $NH_3$ emissions in the NEI are a mix of state-submitted data and EPA estimates. For 2014, the EPA estimates used new methodologies for both livestock and fertilizer emissions. Livestock emissions were estimated based on daily emission factors by animal and county from a model developed by Carnegie Mellon University (CMU) (Pinder, 2004, McQuilling, 2015) and 2012 and 2014 U.S. Department of Agriculture (USDA) agricultural census data. The annual 2014NEIv1 estimates for livestock were updated with revised animal counts for 2014NEIv2 and the resulting 2014NEIv2 numbers for $NH_3$ were used in this study. Although the 2014NEIv2 also includes VOC for livestock, those emission were not used in this study because the numbers had not yet been fully evaluated. For California, state-provided emissions were used for counties and SCCs for which state data were available, while any county-SCC combinations that used EPA data in 2014NEIv1 were updated to use the data from 2014NEIv2. Double-counts between EPA and California data were removed where different SCCs for the same animal type (e.g., beef and swine) were used, with preference given to the California data.

Annual fertilizer emissions were submitted by three states for all or part of the sector as shown in parentheses: California (68 percent), Illinois (100 percent) and Georgia (58 percent). The remainder, estimated by EPA, employed a methodology that uses the bidirectional (bi-di) version of CMAQ and the Fertilizer Emissions Scenario Tool for CMAQ FEST-C (v1.2). This is described in Section 4.4 of the 2014 NEIv1 TSD. These data were used at annual resolution.

### *3.2.3.3 Agricultural fires (ptagfire)*

In the NEI, agricultural fires are stored as county-annual emissions and are part of the nonpoint data category. For this study agricultural fires are modeled as day specific fires derived from satellite data in a similar way to the emissions in ptfire, and state-provided agricultural fire data in AZ, CA, FL, GA, HI, ID, IL, IN, IA, NJ, SC and WA are not used in this study. The first three levels of descriptions for the agricultural burning SCCs are: 1) Fires - Agricultural Field Burning; Miscellaneous Area Sources; 2) Agriculture Production - Crops - as nonpoint; and 3) Agricultural Field Burning - whole field set on fire. The SCC 2801500000 does not specify the crop type or burn method, while the more specific SCCs specify field or orchard crops and, in some cases, the specific crop being grown. New agricultural field burning SCCs were added to the NEI for 2014 to account for grass/pasture burning (also known as rangeland burning) which is included the agriculture field burning sector of the NEI. The EPA's estimation methods were improved from those used in the 2011 NEI and are documented in Section 4.11 of the 2014NEIv1 TSD. Improvements include use of multiple satellite detection database and crop level land use information.

#### *3.2.3.4 Nonpoint Oil-gas Sector (np_oilgas)*

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

An error was discovered in the 2014NEIv1 for nonpoint oil and gas emissions of benzene, ethyl benzene, xylenes and toluene for four counties in the Uinta basin. To compensate for this, emissions from VOC species were genterated using basin specific speciation profiles instead of using the emissions from the inventory. The updates affected the following SCCs: 2310010200 (Oil Well Tanks - Flashing & Standing/Working/Breathing); 2310011201 (Tank Truck/Railcar Loading: Crude Oil); 2310021010 (Storage Tanks: Condensate); and 2310021030 (Tank Truck/Railcar Loading: Condensate), and generally reduced these HAPs from the 2 condensate-related SCCs and increased benzene by a factor of 3 forthe two oil tank-related SCCs. Overall, the np_oilgas emissions in Utah in the platform are 31 tons lower for benzene, 29 tons lower for ethylbenzene, 213 tons lower for toluene, and 335 tons lower for xylenes than the 2014NEIv1.

#### *3.2.3.5 Residential Wood Combustion Sector (rwc)*

The residential wood combustion (rwc) sector includes residential wood burning devices such as fireplaces, fireplaces with inserts (inserts), free standing woodstoves, pellet stoves, outdoor hydronic heaters (also known as outdoor wood boilers), indoor furnaces, and outdoor burning in firepots and chimneas. Free standing woodstoves and inserts are further differentiated into three categories: 1) conventional (not EPA certified); 2) EPA certified, catalytic; and 3) EPA certified, noncatalytic. Generally speaking, the conventional units were constructed prior to 1988. Units constructed after 1988 have to meet EPA emission standards and they are either catalytic or non-catalytic. As with the other nonpoint categories, a mix of S/L and EPA estimates were used. The EPA's estimates use updated methodologies for activity data and some changes to emission factors. For more information on the development of the residential wood combustion emissions, see Section 4.14 of the 2014NEIv1 TSD.

#### *3.2.3.6 Other Nonpoint Sources (nonpt)*

Stationary nonpoint sources that were not subdivided into the afdust, ag, np_oilgas, or rwc sectors were assigned to the "nonpt" sector. Locomotives and CMV mobile sources from the 2014NEIv1 nonpoint inventory are described with the mobile sources. The types of sources in the nonpt sector include:

- stationary source fuel combustion, including industrial, commercial, and residential and orchard heaters;
- chemical manufacturing;
- industrial processes such as commercial cooking, metal production, mineral processes, petroleum refining, wood products, fabricated metals, and refrigeration;
- solvent utilization for surface coatings such as architectural coatings, auto refinishing, traffic marking, textile production, furniture finishing, and coating of paper, plastic, metal, appliances, and motor vehicles;

- solvent utilization for degreasing of furniture, metals, auto repair, electronics, and manufacturing;
- solvent utilization for dry cleaning, graphic arts, plastics, industrial processes, personal care products, household products, adhesives and sealants;
- solvent utilization for asphalt application and roofing, and pesticide application;
- storage and transport of petroleum for uses such as portable gas cans, bulk terminals, gasoline service stations, aviation, and marine vessels;
- storage and transport of chemicals;
- waste disposal, treatment, and recovery via incineration, open burning, landfills, and composting;
- miscellaneous area sources such as cremation, hospitals, lamp breakage, and automotive repair shops.

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

### *3.2.4 Biogenic Sources (beis)*

Biogenic emissions were computed based on the same 14j version of the 2014 meteorology data used for the air quality modeling, and were developed using the Biogenic Emission Inventory System version 3.61 (BEIS3.61) within SMOKE. The BEIS3.61 creates gridded, hourly, model-species emissions from vegetation and soils. It estimates CO, VOC (most notably isoprene, terpene, and sesquiterpene), and NO emissions for the contiguous U.S. and for portions of Mexico and Canada. In the BEIS 3.61 two-layer canopy model, the layer structure varies with light intensity and solar zenith angle (Pouliot and Bash, 2015). Both layers include estimates of sunlit and shaded leaf area based on solar zenith angle and light intensity, direct and diffuse solar radiation, and leaf temperature (Bash et al., 2015). The new algorithm requires additional meteorological variables over previous versions of BEIS. The variables output from the Meteorology-Chemistry Interface Processor (MCIP) that are used to convert WRF outputs to CMAQ inputs are shown in Table 3-5.

**Table 3-5.** Meteorological variables required by BEIS 3.61

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

| Variable | Description |
|---|---|
| TEMPG | skin temperature at ground |
| USTAR | cell averaged friction velocity |
| RADYNI | inverse of aerodynamic resistance |
| TEMP2 | temperature at 2 m |

The BEIS3.61 was used in conjunction with Version 4.1 of the Biogenic Emissions Landuse Database (BELD4.1). The BELD version 4.1 is based on an updated version of the USDA-USFS Forest Inventory and Analysis (FIA) vegetation speciation based data from 2001 to 2014 from the FIA version 5.1. Canopy coverage is based on the Landsat satellite National Land Cover Database (NLCD) product from 2011. The FIA includes approximately 250,000 representative plots of species fraction data that are within approximately 75 km of one another in areas identified as forest by the NLCD canopy coverage. The 2011 NLCD provides land cover information with a native data grid spacing of 30 meters. For land areas outside the conterminous United States, 500 meter grid spacing land cover data from the Moderate Resolution Imaging Spectroradiometer (MODIS) is used. BELDv4.1 also incorporates the following:

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

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

### *3.2.5 Mobile Sources (onroad, onroad_ca_adj, nonroad, cmv_c1c2, cmv_c3, rail)*

Mobile sources are emissions from vehicles that move and include several sectors. Onroad mobile source emissions result from motorized vehicles that are normally operated on public roadways. These include passenger cars, motorcycles, minivans, sport-utility vehicles, light-duty trucks, heavy-duty trucks, and buses. Nonroad mobile source emissions are from vehicles that do not operate on roads such as tractors, construction equipment, lawnmowers, and recreational marine vessels. All nonroad emissions are treated as county-specific low-level emissions (i.e., they are released into model layer 1).

Commercial marine vessel (CMV) emissions are split into two sectors: emissions from Category 1 and Category 2 vessels are in the cmv_c1c2 sector, and emissions from the larger Category 3 vessels are in the cmv_c3 sector where they are treated as point sources with plume rise. Locomotive emissions are in the rail sector. Having the emissions split into these sectors facilitates separating them in summaries and also allows for the largest vessels to be modeled with plume rise.

#### *3.2.5.1 Onroad (onroad)*

Onroad mobile sources include emissions from motorized vehicles that are normally operate on public roadways. These include passenger cars, motorcycles, minivans, sport-utility vehicles, light-duty trucks, heavy-duty trucks, and buses. The sources are further divided between diesel, gasoline, E-85, and compressed natural gas (CNG) vehicles. The sector characterizes emissions from parked vehicle processes (e.g., starts, hot soak, and extended idle) as well as from on-network processes (i.e., from vehicles moving along the roads).

The onroad SCCs in the modeling platform are more finely resolved than those in the NEI, because the NEI SCCs distinguish vehicles and fuels, but in the platform they also distinguish between emissions on roadways, off-network, extended idle, and the various MOVES road-types. For more details on the approach and for a summary of the inputs submitted by states, see the section 6.4.1 of the 2014NEIv1 TSD.

Except for California, onroad emissions are generated using the SMOKE-MOVES interface that leverages MOVES generated emission factors (http://www.epa.gov/otaq/models/moves/index.htm), county and SCC-specific activity data, and hourly meteorological data. SMOKE-MOVES takes into account the temperature sensitivity of the on-road emissions. Specifically, EPA used MOVES inputs for representative counties, vehicle miles traveled (VMT), vehicle population (VPOP), and hoteling hours data for all counties, along with tools that integrated the MOVES model with SMOKE. In this way, it was possible to take advantage of the gridded hourly temperature data available from meteorological modeling that are also used for air quality modeling.

SMOKE-MOVES makes use of emission rate "lookup" tables generated by MOVES that differentiate emissions by process (i.e., running, start, vapor venting, etc.), vehicle type, road type, temperature, speed, hour of day, etc. To generate the MOVES emission rates that could be applied across the U.S., EPA used an automated process to run MOVES to produce year 2014-specific emission factors by temperature and speed for a series of "representative counties," to which every other county was mapped. The representative counties for which emission factors are generated are selected according to their state, elevation, fuels, age distribution, ramp fraction, and inspection and maintenance programs. Each county is then mapped to a representative county based on its similarity to the representative county with respect to those attributes. For this study, there are 297 representative counties. A detailed discussion of the representative counties is in the 2014NEIv1 TSD, Section 6.6.2.

Once representative counties have been identified, emission factors are generated with MOVES for each representative county and for two "fuel months" – January to represent winter months, and July to represent summer months – due to the different types of fuels used. SMOKE selects the appropriate MOVES emissions rates for each county, hourly temperature, SCC, and speed bin and multiplies the emission rate by appropriate activity data. For on-roadway emissions, vehicle miles travelled (VMT) is the activity data, vehicle population (VPOP) is used for many off-network processes, and hoteling hours are used to develop emissions for extended idling of combination long-haul trucks. These calculations are done for every county and grid cell in the continental U.S. for each hour of the year.

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

1) Determine which counties will be used to represent other counties in the MOVES runs.
2) Determine which months will be used to represent other month's fuel characteristics.
3) Create inputs needed only by MOVES. MOVES requires county-specific information on vehicle populations, age distributions, and inspection-maintenance programs for each of the representative counties.
4) Create inputs needed both by MOVES and by SMOKE, including temperatures and activity data.
5) Run MOVES to create emission factor tables for the temperatures found in each county.

6) Run SMOKE to apply the emission factors to activity data (VMT, VPOP, and HOTELING) to calculate emissions based on the gridded hourly temperatures in the meteorological data.
7) Aggregate the results to the county-SCC level for summaries and quality assurance.

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

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

The onroad emissions inputs for the platform are the same as for the emissions in the onroad data category of the 2014NEIv1, described in more detail in Sections 6.4 and 6.5 of the 2014NEIv1 TSD. These inputs are:

- MOVES County databases (CDBs) including Low Emission Vehicle (LEV) table
- Representative counties
- Fuel months
- Meteorology
- Activity data (VMT, VPOP, speed, HOTELING)

An additional step was taken for the refueling emissions. Colorado submitted point emissions for refueling for some counties[7]. For these counties, the EPA zeroed out the onroad estimates of refueling (i.e., SCCs =220xxxxx62) so that the states' point emissions would take precedence. The onroad refueling emissions were zeroed out using the adjustment factor file (CFPRO) and Movesmrg.
For more detailed information on the methods used to develop the 2014 onroad mobile source emissions and the input data sets, see Section 6.6 of the 2014NEIv1 TSD.

California is the only state agency for which submitted onroad emissions were used in the 2014 NEI v1 and 2014v7.0 platform. California uses their own emission model, EMFAC, which uses emission inventory codes (EICs) to characterize the emission processes instead of SCCs. The EPA and California worked together to develop a code mapping to better match EMFAC's EICs to EPA MOVES' detailed set of SCCs that distinguish between off-network and on-network and brake and tire wear emissions. This detail is needed for modeling but not for the NEI. This code mapping is provided in "2014v1_EICtoEPA_SCCmapping.xlsx." California then provided their CAP and HAP emissions by county using EPA SCCs after applying the mapping. There was one change made after the mapping: the vehicle/fuel type combination gas intercity buses (first 6 digits of the SCC = 220141), that is not

7 There were 52 counties in Colorado that had point emissions for refueling. Outside Colorado, it was determined that refueling emissions in the 2014 NEIv1 point did not significantly duplicate the refueling emissions in onroad.

generated using MOVES, was changed to gasoline single unit short-haul trucks (220152) for consistency with the modeling inventory.

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

1) Run CA using EPA inputs through SMOKE-MOVES to produce hourly 2014 emissions hereafter known as "EPA estimates." These EPA estimates for CA are run in a separate sector called "onroad_ca."
2) Calculate ratios between state-supplied emissions and EPA estimates. These were calculated for each county/SCC/pollutant combination. Unlike in previous platforms, the California data separated off and on-network emissions and extended idling. However, the on-network did not provide specific road types, and California's emissions did not include information for vehicles fueled by E-85, so these differentiations were obtained using MOVES.
3) Create an adjustment factor file (CFPRO) that includes EPA-to-state estimate ratios.
4) Rerun CA through SMOKE-MOVES using EPA inputs and the new adjustment factor file.

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

#### *3.2.5.2 MOVES-based Nonroad Mobile Sources (nonroad)*

The nonroad equipment emissions in the platform and the NEI result primarily from running the MOVES2014a model, which incorporates the NONROAD2008 model. MOVES2014a replaces NMIM, which was used for 2011 and earlier NEIs. MOVES2014a provides a complete set of HAPs and incorporates updated nonroad emission factors for HAPs. MOVES2014a was used for all states other than California, which uses their own model. Additional details on the development of the 2014NEIv1 nonroad emissions are available in Section 4.5 the 2014NEIv1 TSD.

The magnitude of the annual emissions in the nonroad platform are equivalent to the emissions in the nonroad data category of the 2014NEIv1. However, the platform has monthly emission totals, which are provided by MOVES2014a and contain additional pollutants used in the emissions modeling. The emissions in the modeling platform include NONHAPTOG and ETHANOL, which are not included in the NEI. NONHAPTOG is the difference between total organic gases (TOG) and explicit species that are estimated separately such as benzene, toluene, styrene, ethanol, and numerous other compounds and are integrated into the chemical speciation process. MOVES2014a provides estimates of NONHAPTOG along with the speciation profile code for the NONHAPTOG emission source. This is accomplished by using NONHAPTOG#### as the pollutant code in the FF10 inventory file, where #### is a speciation profile code. Since speciation profiles are applied by SCC and pollutant, no changes to SMOKE were needed in order to use the FF10 with this profile information. This approach is not used for California,

because their model provides VOC and traditional speciation is performed in SMOKE instead.

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

#### *3.2.5.3 Locomotive (rail)*

The rail sector includes all locomotives in the NEI nonpoint data category. This sector excludes railway maintenance locomotives and point source yard locomotives. Railway maintenance emissions are included in the nonroad sector. The point source yard locomotives are included in the ptnonipm sector. The nonpoint rail data are a mix of S/L and EPA data. For 2014NEIv1, the EPA data were carried forward from the 2011 NEI. For more information on locomotive sources in the NEI, see Section 4.20 of the 2014NEIv1 TSD.

#### *3.2.5.4 Category 1, 2, and 3 commercial marine vessels (cmv_c1c2 and cmv_3)*

The cmv_c1c2 sector contains Category 1 and 2 CMV emissions from the 2014 NEIv1. Category 1 and 2 vessels use diesel fuel. All emissions in this sector are annual and at county-SCC resolution; however, in the NEI they are provided at the sub-county level (port or underway shape ids) and by SCC and emission type (e.g., hoteling, maneuvering). This sub-county data in the NEI are used to create spatial surrogates. The emissions for the CMV sector are equivalent to those in the 2014NEIv1 nonpoint inventory. For more information on CMV sources in the NEI, see Section 4.3 of the 2014NEIv1 TSD. C1 and C2 emissions that occur outside of state waters are not assigned to states. All CMV emissions in the cmv_c1c2 sector are treated as nonpoint sources, and are placed in layer 1 and allocated to grid cells using spatial surrogates.

The Category 3 CMV vessels in the cmv_c3 sector use residual oil. The cmv_c3 sector uses 2014NEIv1 emissions in state waters but excludes NEI C3 emissions in Federal Waters (FIPS codes beginning with 85). Instead, more spatially resolved emissions from the Emissions Control Area-International Marine Organization (ECA-IMO)-based C3 CMV are used. The C3 CMV emissions are treated as point sources and were developed based on a 4-km resolution ASCII raster format dataset that preserves shipping lanes and extends within and beyond the federal waters. The treatment of these emissions as point sources allows for them to have plume rise when modeled by SMOKE and CMAQ. This dataset has been used since the Emissions Control Area-International Marine Organization (ECA-IMO) project began in 2005, although it was then known as the Sulfur Emissions Control Area (SECA). The ECA-IMO emissions consist of large marine diesel engines (at or above 30 liters/cylinder) that until recently were allowed to meet relatively modest emission requirements and as a result these ships would often burn residual fuel in that region. The emissions in this sector are comprised of primarily foreign-flagged ocean-going vessels, referred to as C3 CMV ships. The C3 portion of the CMV inventory includes these ships in several intra-port modes (i.e., cruising, hoteling, reduced speed zone, maneuvering, and idling) and an underway mode, and includes near-port auxiliary engine emissions.

An overview of the C3 ECA Proposal to the International Maritime Organization (EPA-420-F-10-041, August 2010) project and future-year goals for reduction of $NO_X$, $SO_2$, and PM C3 emissions can be found at: http://www.epa.gov/oms/regs/nonroad/marine/ci/420r09019.pdf. The resulting ECA-IMO coordinated strategy, including emission standards under the Clean Air Act for new marine diesel engines with per-cylinder displacement at or above 30 liters, and the establishment of Emission Control Areas is available from https://www.epa.gov/regulations-emissions-vehicles-and-engines/international-standards-reduce-emissions-marine-diesel. The base year for the ECA inventory is 2002 and consists of these CAPs: $PM_{10}$, $PM_{2.5}$, CO, $CO_2$, $NH_3$, $NO_X$, $SO_X$ (assumed to be $SO_2$), and hydrocarbons (assumed to be VOC). EPA developed regional growth (activity-based) factors that were applied to create the 2012 inventory from the 2002 data. The geographic regions listed in the table are shown in Figure 31.

* Technically, these are not really "FIPS" state-county codes, but are treated as such in the inventory and emissions processing.

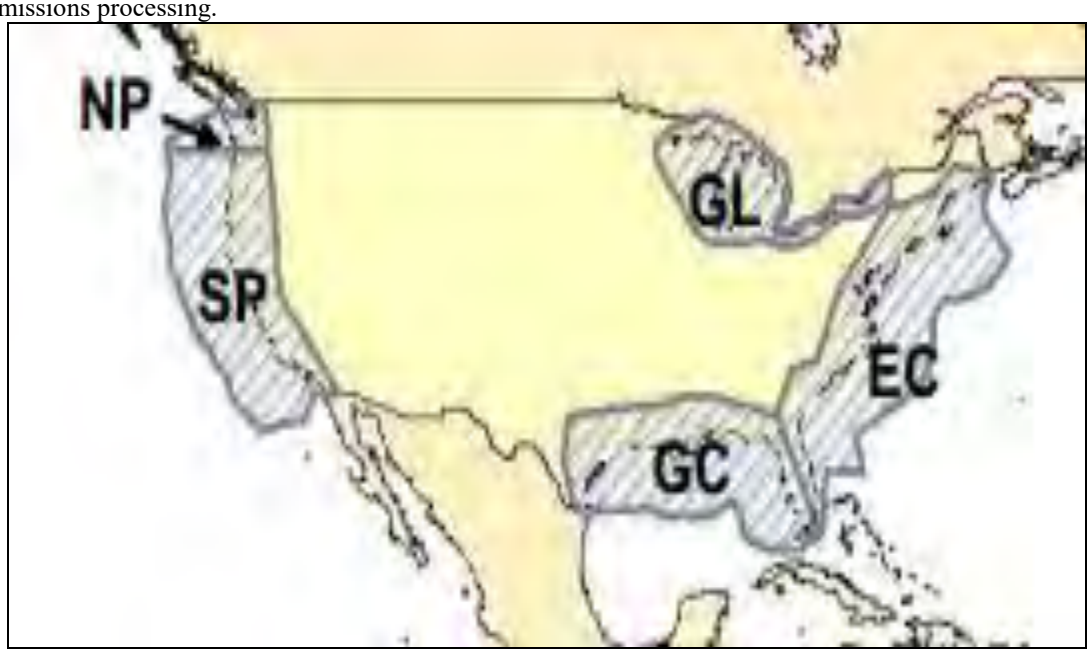


**Figure 3-1. Illustration of regional modeling domains in ECA-IMO study**

The East Coast and Gulf Coast regions were divided along a line roughly through Key Largo (longitude 80° 26' West). Technically, the EEZ FIPS are not really "FIPS" state-county codes, but are treated as such in the inventory and emissions processing. The Canadian near-shore emissions were assigned to province-level FIPS codes and paired those to region classifications for British Columbia (North Pacific), Ontario (Great Lakes) and Nova Scotia (East Coast).

The emissions were converted to SMOKE point source inventory format as described in https://www3.epa.gov/ttn/chief/conference/ei17/session6/mason.pdf, which allows for the emissions to be allocated to modeling layers above the surface layer. As described in the paper, the ASCII raster dataset was converted to latitude-longitude, mapped to state/county FIPS codes that extended up to 200 nautical miles (nm) from the coast, assigned stack parameters, and monthly ASCII raster dataset emissions were used to create monthly temporal profiles. All non-US, non-EEZ emissions (i.e., in waters considered outside of the 200 nm EEZ, and hence out of the U.S. and Canadian ECA-IMO controllable domain) were simply assigned a dummy state/county FIPS code=98001, and were projected to year 2011 using the "Outside ECA" factors. Note that the year 2011 emissions were used for this 2014 study.

The assignment of U.S. state/county FIPS codes was restricted to state-federal water boundaries data from the Mineral Management Service (MMS) that extend approximately 3 to 10 nautical miles (nm) off shore. Emissions outside the 3 to 10 mile MMS boundary, but within the approximately 200 nm EEZ boundaries in Figure 3-1, were projected to year 2011 using the same regional adjustment factors as the U.S. emissions; however, the state/county FIPS codes were assigned as "EEZ" codes and those emissions processed in the "othpt" sector. Note that state boundaries in the Great Lakes are an exception, extending through the middle of each lake such that all emissions in the Great Lakes are assigned to a U.S. county or Ontario. This holds true for Midwest states and other states such as Pennsylvania and New York. The classification of emissions to U.S. and Canadian FIPS codes was needed to avoid double-counting of C3 CMV U.S. emissions in the Great Lakes, because all CMV emissions in the Midwest RPO are classified as C1 or C2 sources in the CMV inventory.

The SMOKE-ready data have been cropped from the original ECA-IMO entire northwestern quarter of the globe to cover only the large continental U.S. 36-km "36US1" air quality model domain, the largest domain used by EPA in recent years.

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

For California, the ECA-IMO 2014 emissions were scaled to match those provided by CARB for the 2014NEIv1. Note that CARB has had distinct projection and control approaches for this sector since 2002. These CARB C3 CMV emissions are documented in a staff report available at: http://www.arb.ca.gov/regact/2010/offroadlsi10/offroadisor.pdf. The CMV emissions obtained from CARB include the 2014 regulations to reduce emissions from diesel engines on commercial harbor craft operated within California waters and 24 nautical miles of the California shoreline.

### *3.2.6 Emissions from Canada, Mexico (othpt, othar, othafdust, onroad_can, onroad_mex, ptfire_mxca)*

The emissions from Canada, Mexico, and non-U.S. offshore Category 3 CMV (C3 CMV) and drilling platforms are included as part of the emissions modeling sectors: othpt, othar, othafdust, onroad_can, and onroad_mex. The "oth" refers to the fact that these emissions are usually "other" than those in the U.S. state-county geographic FIPS, and the remaining characters provide the SMOKE source types: "pt" for point, "ar" for area and nonroad mobile, "afdust" for area fugitive dust (Canada only). The onroad emissions for Canada and Mexico are in the onroad_can and onroad_mex sectors, respectively.

For Canadian point sources, 2013 emissions provided by Environment Canada were used. These included VOC emissions and CB6 speciation for VOCs although the CB6 VOCs differed slightly from the version of CB6 in CMAQ. Airport emissions were provided by month. Temporal profiles were provided for all source categories. Point sources in Mexico were compiled based on a year 2014 inventory projected from the the Inventario Nacional de Emisiones de Mexico, 2008 (ERG, 2014a; ERG, 2016a). The point source emissions in the 2014 inventory were converted to English units and into the FF10 format that could be read by SMOKE, missing stack parameters were gapfilled using SCC-based defaults, and latitude and longitude coordinates were verified and adjusted if they were not consistent with the reported municipality. Note that there are no explicit HAP emissions in this inventory.

For Canadian area and nonroad sources, year-2013 emissions provided by Environment Canada were used, including CMV emissions. The Canadian inventory included fugitive dust emissions that do not incorporate either a transportable fraction or meteorological-based adjustments. To properly account for this, a separate sector called othafdust was created and modeled using the same adjustments as are done for U.S. sources. Updated Shapefiles used for creating spatial surrogates for Canada were also provided. For Canada nonroad mobile sources, the provided 2013 monthly emissions were used.

For Canada onroad emissions, month-specific year-2013 emissions provided by Environment Canada were used. Note that unlike the U.S. and Mexico inventories, there are no explicit HAPs in the onroad inventories for Canada and, therefore, NBAFM HAPs are created from speciation. For Mexico onroad emissiosn, a version of the MOVES model for Mexico was run that provided the same VOC HAPs and speciated VOCs as for the U.S. MOVES model (ERG, 2016a). This includes NBAFM plus several other VOC HAPs such as toluene, xylene, ethylbenzene and others. Except for VOC HAPs that are part of the speciation, no other HAPs are included in the Mexico onroad inventory (such as particulate HAPs nor diesel particulate matter).

Annual 2014 wildland emissions for Mexico and Canada are in the ptfire_mxca sector. They were developed from a combination of Fire Inventory from NCAR (FINN) daily fire emissions and fire data provided by Environment Canada for the months of June through November and FINN fire emissions were used to fill in the annual gaps from January through May and December. The FINN fire emissions come from an updated FINN v1.5 data set that differs from previous 2014 platforms largely in the inclusion of grassland and cropland coverage. Only CAP emissions are provided in the Canada and Mexico fire inventories. For FINN fires, listed vegetation type codes of 1 and 9 are defined as agricultural burning, all other fire detections and assumed to be wildfires. All wildland fires that are not defined as agricultural are assumed to be wild fires rather than prescribed. FINN fire detects less than 50 square meters (0.012 acres) are removed from the inventory. The locations of FINN fires are geocoded from latitude and longitude to FIPS code.

### *3.2.7 SMOKE-ready non-anthropogenic chlorine inventory*

The ocean chlorine gas emission estimates are based on the build-up of molecular chlorine (Cl2) concentrations in oceanic air masses (Bullock and Brehme, 2002). Data at 36 km and 12 km resolution were available and were not modified other than the name “CHLORINE” was changed to “CL2” because that is the name required by the CMAQ model.

## 3.3 Emissions Modeling Summary

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

As previously discussed, 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.

### *3.3.1 The SMOKE Modeling System*

SMOKE version 4.5 was used to pre-process the raw emissions inventories into emissions inputs for CMAQ. SMOKE executables and source code are available from the Community Multiscale Analysis System (CMAS) Center at http://www.cmascenter.org. Additional information about SMOKE is available from http://www.smoke-model.org. For sectors that have plume rise, the in-line emissions capability of the air quality models was used, which allows the creation of source-based and two-dimensional gridded emissions files that are much smaller than full three-dimensional gridded emissions files. For quality assurance of the emissions modeling steps, emissions totals by specie for the entire model domain are output as reports that are then compared to reports generated by SMOKE on the input inventories to ensure that mass is not lost or gained during the emissions modeling process.

### *3.3.2 Key Emissions Modeling Settings*

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 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 3-6 summarizes the major processing steps of each platform sector. The "Spatial" column shows the spatial approach used: here "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. 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.

**Table 3-6.** Key emissions modeling steps by sector

| Platform sector | Spatial | Speciation | Inventory resolution | Plume rise |
|---|---|---|---|---|
| afdust_adj | Surrogates | Yes | annual | |
| ag | Surrogates | Yes | annual | |
| beis | Pre-gridded land use | in BEIS | 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 | |

| Platform sector | Spatial | Speciation | Inventory resolution | Plume rise |
|---|---|---|---|---|
| np_oilgas | Surrogates | Yes | annual | |
| onroad | Surrogates | Yes | monthly activity, computed hourly | |
| onroad_ca_adj | Surrogates | Yes | monthly activity, computed hourly | |
| onroad_can | Surrogates | Yes | Monthly | |
| onroad_mex | Surrogates | Yes | Monthly | |
| othafdust | Surrogates | Yes | Annual | |
| othar | Surrogates | Yes | annual & monthly | |
| othpt | Point | Yes | annual & monthly | in-line |
| ptagfire | Point | Yes | Daily | none |
| pt_oilgas | Point | Yes | Annual | in-line |
| ptegu | Point | Yes | daily & hourly | in-line |
| ptfire | Point | Yes | Daily | in-line |
| ptfire_mxca | 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 study, the in-line biogenic emissions option was used, and so biogenic emissions from BEIS were not included in the gridded CMAQ-ready emissions.

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 the stack data and the hourly air quality model inputs found in the SMOKE output files for each model-ready emissions sector. The height of the plume rise determines the model layer into which the emissions are placed. The cmv_c3, othpt, ptfire, and ptfire_mxca sectors have 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. Day-specific point fires are treated separately for CMAQ modeling in that fire plume rise is done within CMAQ itself. After plume rise is applied, there will be emissions in every layer from the ground up to the top of the plume. For the ptagfire sector, all emissions were allocated to layer 1 and output to gridded 2-D emissions files.

SMOKE has the option of grouping sources so that they are treated as a single stack when computing plume rise. For the 2014 modeling case, 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 lat/lons 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.

### *3.3.3 Spatial Configuration*

For this study, SMOKE was run for the larger 12-km CONtinental United States "CONUS" modeling domain (12US1) shown in Figure 3-2 and boundary conditions were obtained from a 2014 run of GEOS-Chem. The grid used a Lambert-Conformal projection, with Alpha = 33, Beta = 45 and Gamma = -97, with a center of X = -97 and Y = 40. Later sections provide details on the spatial surrogates and area-to-point data used to accomplish spatial allocation with SMOKE.

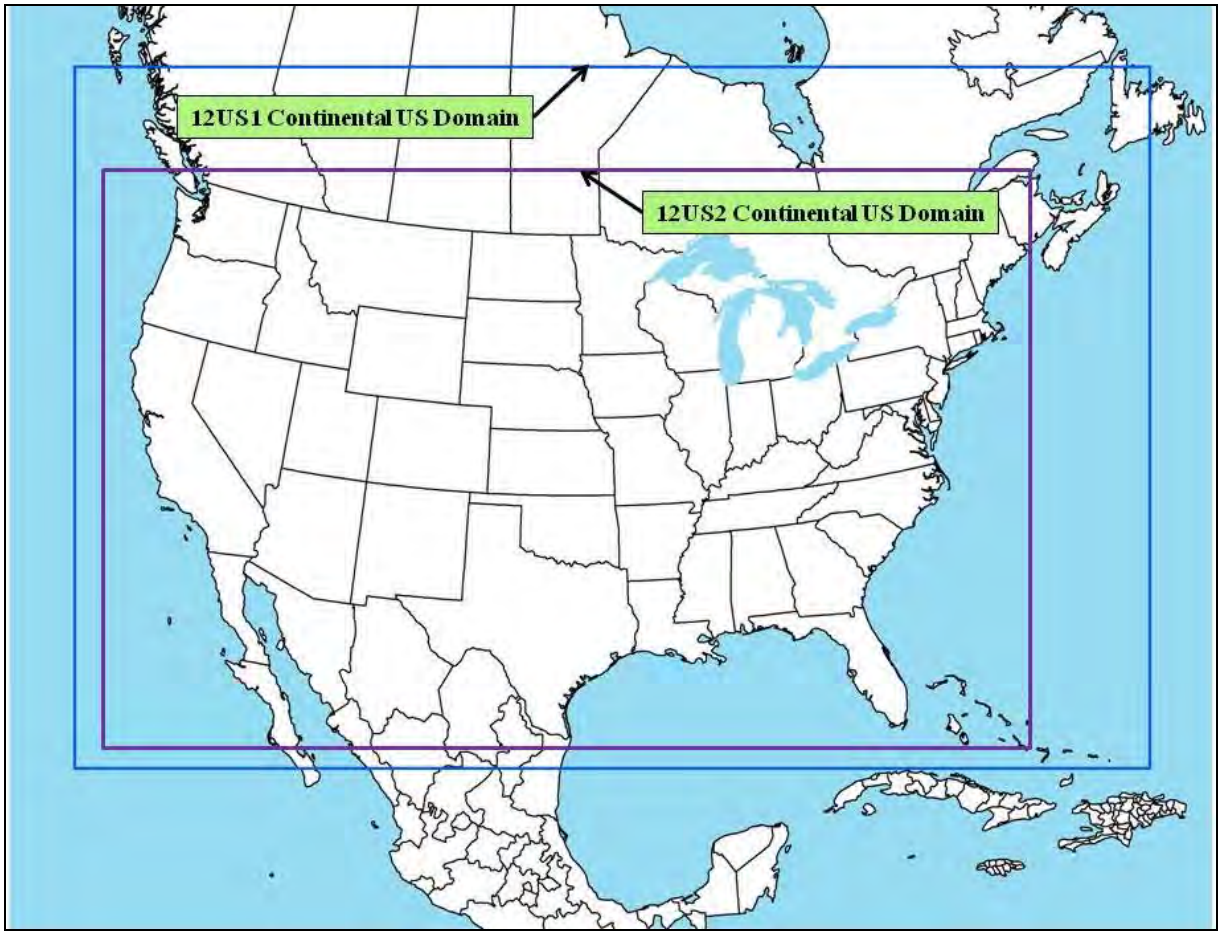


**Figure 3-2. CMAQ Modeling Domain**

### *3.3.4 Chemical Speciation Configuration*

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 2014 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 3-7 lists the model species produced by SMOKE in the platform used for this study.

**Table 3-7. 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 |

| Inventory Pollutant | Model Species | Model species description |
|---|---|---|
| | PCA | Calcium |
| | PCL | Chloride |
| | PFE | Iron |
| | PK | Potassium |
| | PH2O | Water |
| | PMG | Magnesium |
| | PMN | Manganese |
| | PMOTHR | $PM_{2.5}$ not in other AE6 species |
| | PNA | Sodium |
| | PNCOM | Non-carbon organic matter |
| | PNH4 | Ammonium |
| | PSI | Silica |
| | PTI | Titanium |
| Sea-salt species (non – anthropogenic) [8] | 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-version-45-through-40), which is the EPA's repository of TOG and PM speciation profiles of air pollution sources. The SPECIATE database development and maintenance is a collaboration involving the EPA's Office of Research and Development (ORD), Office of Transportation and Air Quality (OTAQ), and the Office of Air Quality Planning and Standards (OAQPS), in cooperation with Environment Canada (EPA, 2016). The SPECIATE database contains speciation profiles for TOG, speciated into individual chemical compounds, VOC-to-TOG conversion factors associated with the TOG profiles, and speciation profiles for $PM_{2.5}$.

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

- VOC speciation profile cross reference assignments for point and nonpoint oil and gas sources were updated to (1) make corrections to 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;
- Two new $PM_{2.5}$ profiles from SPECIATE4.5 are used for brake and tirewear;
- speciation profiles developed by the Western Regional Air Partnership (WRAP) are used for the np_oilgas sector were revised;
- VOC speciation for nonroad mobile has been updated to include a different speciation profile assignment method for VOC (profiles are assigned to SCCs within MOVES2014a which outputs the emissions with those assignments) and updated profiles;

[8] These emissions are created outside of SMOKE

- VOC and PM speciation for onroad mobile sources occurs within MOVES2014a;
- Speciation for onroad mobile sources in Mexico is done within MOVES and is more consistent with that used in the United States; and
- The 2013 Canadian point source inventories were provided from Environment Canada with CB6 speciation.

Speciation profiles and cross-references for the 2014 platform are available in the SMOKE input files for the 2014 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 Appendix B state-sector totals workbook for this case.

The speciation of VOC includes HAP emissions from the 2014NEIv1 in the speciation process. Instead of speciating VOC to generate all of the species listed in Table 3-7, 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 other than PTDAY (the format used for the ptfire sector). SMOKE allows the user to specify both 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[9]). 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[10]. SMOKE computes NONHAPTOG and then applies the speciation profiles to allocate the NONHAPTOG to the other air quality model VOC species not including the integrated HAPs. After determining if a sector is to be integrated, if all sources have the appropriate HAP emissions, then the sector is considered fully integrated and does not need a NHAPEXCLUDE file. If, on the other hand, certain sources do not have

9 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.

10 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.

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 3-3). 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 3-3 illustrates the integrate and no-integrate processes for U.S. Sources. Since Canada and Mexico inventories do not contain HAPs, we use the 2011v6.3 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. These profiles are listed in Appendix E. 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 3-8), 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 four 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.

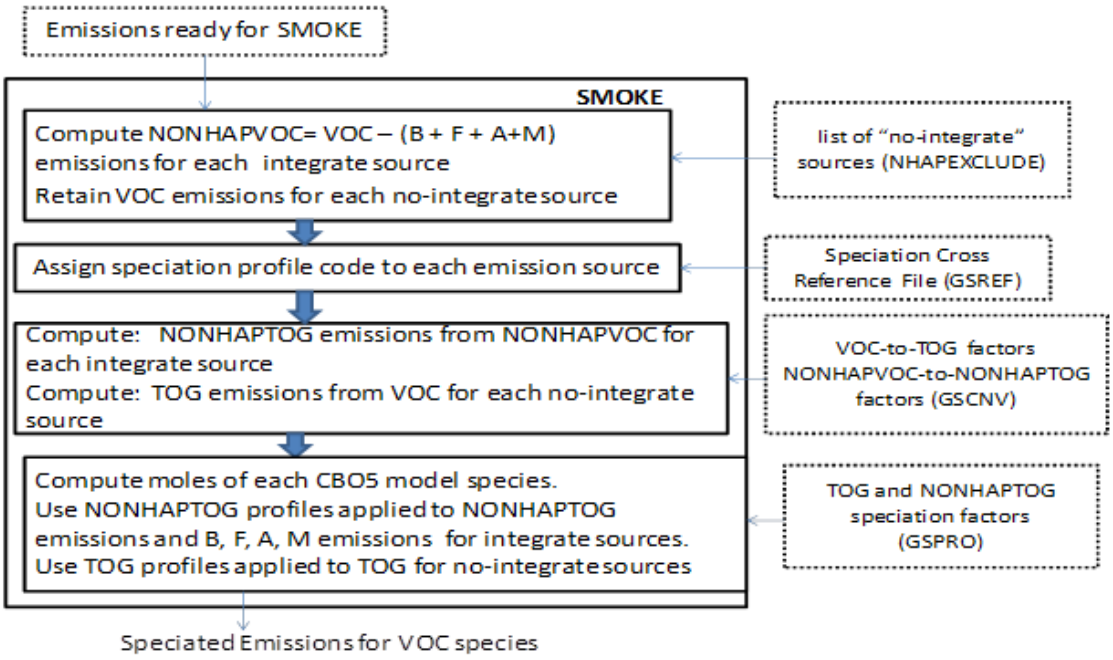


**Figure 3-3**. Process of integrating BAFM with VOC for use in VOC Speciation

**Table 3-8. Integration status of benzene, acetaldehyde, formaldehyde and methanol (BAFM) 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, create NBAFM from VOC speciation |
| ptfire_mxca | No integration, create NBAFM from VOC speciation |
| ptagfire | No integration, create NBAFM from VOC speciation |
| ag | N/A – sector contains no VOC |
| 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, create NBAFM from VOC speciation |
| pt_oilgas | No integration, create NBAFM from VOC speciation |
| rwc | Partial integration (NBAFM) |
| onroad | Full integration (internal to MOVES) |
| onroad_can | No integration, no NBAFM in inventory, create NBAFM from speciation |
| onroad_mex | Full integration (internal to MOVES-Mexico); however, MOVES-MEXICO speciation |

| Platform Sector | Approach for Integrating NEI emissions of Naphthalene (N), Benzene (B), Acetaldehyde (A), Formaldehyde (F) and Methanol (M) |
|---|---|
| | was CB6-CAMx, not CB6-CMAQ, so post-SMOKE emissions were converted to CB6-CMAQ |
| othafdust | N/A – sector contains no VOC |
| othar | No integration, 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. 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.

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 varies 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 allows combinations to be specified at various levels for different years. For the 2014v7.0 platform, GSPRO_COMBO is still used for nonroad sources in California and for certain gasoline-related stationary sources nationwide. The feature is also used to combine exhaust and evaporative profiles to use with Mexican nonroad sources, which do not include the mode in the SCC or pollutant. GSPRO_COMBO is no longer needed for nonroad sources in the US 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.

A new method to combine multiple profiles is available in SMOKE4.5. It allows multiple profiles to be combined by 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.

Speciation profiles for use with BEIS are not included in SPECIATE. BEIS3.61 includes a species (SESQ) that was mapped to the CMAQ specie SESQT. The profile code associated with BEIS profiles for use with CB6 was "B10C6." For additional sector-specific details on VOC speciation for a variety of sectors, see Section 3.2.1.3 of the 2011v6.2 TSD (EPA, 2015a).

In addition to VOC profiles, the SPECIATE database also contains the $PM_{2.5}$ speciated into both individual chemical compounds (e.g., zinc, potassium, manganese, lead), and into the "simplified" $PM_{2.5}$ components used in the air quality model. For CMAQ 4.7.1 modeling, these "simplified" components (AE5) are all that is needed. Starting with CMAQ 5.0.1, a new thermodynamic equilibrium aerosol modeling tool (ISORROPIA) v2 mechanism was added that needs additional PM components (AE6),

which are further subsets of PMFINE (see Table 3-9). The majority of the 2014 platform PM profiles come from the 911XX series which include updated AE6 speciation[11].

**Table 3-9. PM model species: AE5 versus AE6**

| Species name | Species description | AE5 | AE6 |
|---|---|---|---|
| POC | organic carbon | Y | Y |
| PEC | elemental carbon | Y | Y |
| PSO4 | Sulfate | Y | Y |
| PNO3 | Nitrate | Y | Y |
| PMFINE | unspeciated $PM_{2.5}$ | Y | N |
| PNH4 | Ammonium | N | Y |
| PNCOM | non-carbon organic matter | N | Y |
| PFE | Iron | N | Y |
| PAL | Aluminum | N | Y |
| PSI | Silica | N | Y |
| PTI | Titanium | N | Y |
| PCA | Calcium | N | Y |
| PMG | Magnesium | N | Y |
| PK | Potassium | N | Y |
| PMN | Manganese | N | Y |
| PNA | Sodium | N | Y |
| PCL | Chloride | N | Y |
| PH2O | Water | N | Y |
| PMOTHR | $PM_{2.5}$ not in other AE6 species | N | Y |

Unlike other sectors, the onroad sector has pre-speciated PM. This speciated PM comes from the MOVES model and is processed through the SMOKE-MOVES system. Unfortunately, the MOVES speciated PM does not map one-to-one to the AE5 speciation (nor the AE6 speciation) needed for CMAQ modeling. For additional details on PM speciation, see Section 3.2.2 of the 2011v6.2 platform TSD (EPA, 2015a).

$NO_X$ can be speciated into NO, NO2, and/or HONO. For the non-mobile sources, EPA used a single profile "NHONO" to split $NO_X$ into NO and $NO_2$. For the mobile sources except for onroad (including nonroad, cmv_c1c2, cmv_c3, rail, onroad_can, onroad_mex sectors) and for specific SCCs in othar and ptnonipm, the profile "HONO" splits $NO_X$ into NO, $NO_2$, and HONO. Table 3-10 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

[11] The exceptions are 5674 (Marine Vessel – Marine Engine – Heavy Fuel Oil) used for c3marine and 92018 (Draft Cigarette Smoke – Simplified) used in nonpt.

year and equals 1 – NO – HONO. For more details on the $NO_X$ fractions within MOVES, see http://www.epa.gov/otaq/models/moves/documents/420r12022.pdf.

**Table 3-10.** $NO_X$ 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 |

Additional details on speciation for onroad, nonroad, and oil and gas sources, and new PM profiles used are discussed in the 2014v7.0 TSD (EPA, 2017a).

### *3.3.5 Temporal Processing Configuration*

Temporal allocation (i.e., temporalization) is the process of distributing aggregated emissions to a finer temporal resolution, thereby converting annual emissions to hourly emissions. 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. Temporalization takes these aggregated emissions and, if needed, distributes them to the month, and then distributes the monthly emissions to the day and the daily 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.

The temporal factors applied to the inventory are selected using some combination of country, state, county, SCC, and pollutant. Table 3-11 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 3-11. 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 | Annual | Yes | met-based | all | Yes |
| beis | Hourly | | n/a | all | Yes |
| cmv_c1c2 | Annual | Yes | aveday | aveday | |
| cmv_c3 | Annual | Yes | aveday | aveday | |
| nonpt | Annual | Yes | week | week | Yes |
| nonroad | Monthly | | mwdss | Mwdss | Yes |

| Platform sector short name | Inventory resolutions | Monthly profiles used? | Daily temporal approach | Merge processing approach | Process Holidays as separate days |
|---|---|---|---|---|---|
| np_oilgas | Annual | yes | week | week | Yes |
| onroad | Annual & monthly[1] | | all | all | Yes |
| onroad_ca_adj | Annual & monthly[1] | | all | all | Yes |
| othafdust_adj | Annual | yes | week | week | |
| othar | Annual & monthly | yes | week | week | |
| onroad_can | Monthly | | week | week | |
| onroad_mex | Monthly | | week | week | |
| othpt | Annual & monthly | yes | mwdss | mwdss | |
| ptagfire | Daily | | all | all | Yes |
| pt_oilgas | Annual | yes | mwdss | mwdss | Yes |
| ptegu | Daily & hourly | | all | all | Yes |
| ptnonipm | Annual | yes | mwdss | mwdss | Yes |
| ptfire | Daily | | all | all | Yes |
| ptfire_mxca | Daily | | all | all | Yes |
| rail | Annual | yes | aveday | aveday | |
| rwc | Annual | no | met-based | all | Yes |

1. Note the annual and monthly "inventory" actually refers to the activity data (VMT and VPOP) for onroad. The actual emissions are computed on an hourly basis.

The following values are used in Table 3-11: 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 temporalization 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, 2014, which is intended to mitigate the effects of initial condition concentrations. The ramp-up period was 10 days (December 22-31, 2013). For all anthropogenic sectors, emissions from December 2014 were used to fill in surrogate emissions for the end of December 2013. In particular, December 2014 emissions (representative days) were used for December 2013. For biogenic emissions, December 2013 emissions were processed using 2013 meteorology.

The Flat File 2010 format (FF10) inventory format for SMOKE provides a more consolidated format for monthly, daily, and hourly emissions inventories than prior formats supported. Previously, processing monthly inventory data required the use of 12 separate inventory files. 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 temporalization applied to it; rather, it should only have month-to-day and diurnal temporalization. This becomes particularly important when specific sectors have a mix of annual, monthly, daily, and/or hourly inventories. The flags that control temporalization 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 nonroad, onroad (for activity data), onroad_can, onroad_mex, othar, othpt, and ptegu.

#### *3.3.5.1 Standard Temporal Profiles*

Some sectors use straightforward temporal profiles not based on meteorology or other factors. For the ptagfire sector, the inventories are in the daily point fire format, so temporal profiles are only used to go from day-specific to hourly emissions. For all agricultural burning, the diurnal temporal profile used reflected the fact that burning occurs during the daylight. This puts most of the emissions during the work day and suppresses the emissions during the middle of the night. This diurnal profile was used for each day of the week for all agricultural burning emissions in all states.

For the cmv_c1c2 and cmv_c3 sectors, emissions are allocated with flat day of week and flat hourly profiles. The C1 and C2 emissions are allocated with a flat monthly profile, except in the Great Lakes, where the profiles vary by month. C3 emissions are allocated with monthly profiles developed specifically for C3, including in the Great Lakes.

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

For the ptfire sector, the inventories are in the daily point fire format, so temporal profiles are only used to go from day-specific to hourly emissions. For the nonroad sector, while the NEI only stores the annual totals, the modeling platform uses monthly inventories from output from NMIM. For California, the nonroad inventory is annual only, and monthly temporal profiles are applied in SMOKE.

Diurnal, weekly, and monthly temporal profiles for aviation-related sources were updated in the 2014v7.0 platform based on aviation metrics. Details on these new profiles are available in the 2014v7.0 TSD. Temporal profiles for small airports (i.e., non-commercial) do not have any emissions between 10pm and 6am due to a lack of tower operations. Industrial processes that are not likely to shut down on Sundays such as those at cement plants are assigned to other more realistic profiles that included emissions on Sundays. This also affected emissions on holidays because Sunday emissions are also used on holidays.

For oil and gas sources, monthly profiles were applied based on monthly activity data computed from the data sources used to develop the 2014 NEI. The profiles were specific to each FIPS and SCC and were applied as part of the cross reference. For states that used non-standard SCCs not in the EPA data set, flat profiles were used. Many np_oilgas sources use profiles that represent 24 hours per day, 7 days a week.

For agricultural livestock, annual-to-month profiles were developed based on daily emissions data output

from the CMU model by state and SCC. These profiles were used to temporally allocate 2014NEIv2 ag livestock emissions to monthly emissions, which are further temporally allocated to hours as described below in section 3.3.5.3.

#### *3.3.5.2 Temporal Profiles for EGUs*

The 2014NEIv1 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 3-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 cause erroneously high values in the CEMS data. If the data were not measured at specific hours, and those values were found to be more than three times the annual mean for that unit, the data for those hours were replaced with annual mean values (Adelman et al., 2012). These adjusted CEMS data were then used for the remainder of the temporalization process described below (see Figure 3-4 Figure 3-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 3-5.

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 may be different than the annual values in 2014NEIv1 because the CEMS data actually replaces the 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.

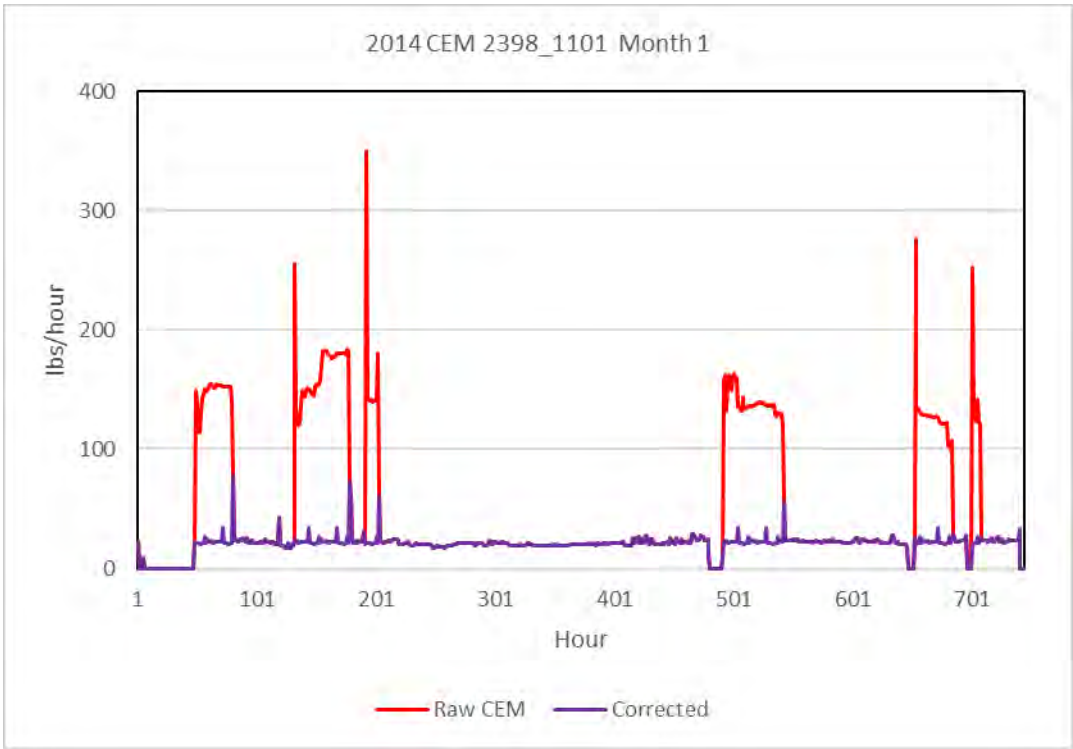


**Figure 3-4.** Eliminating unmeasured spikes in CEMS data

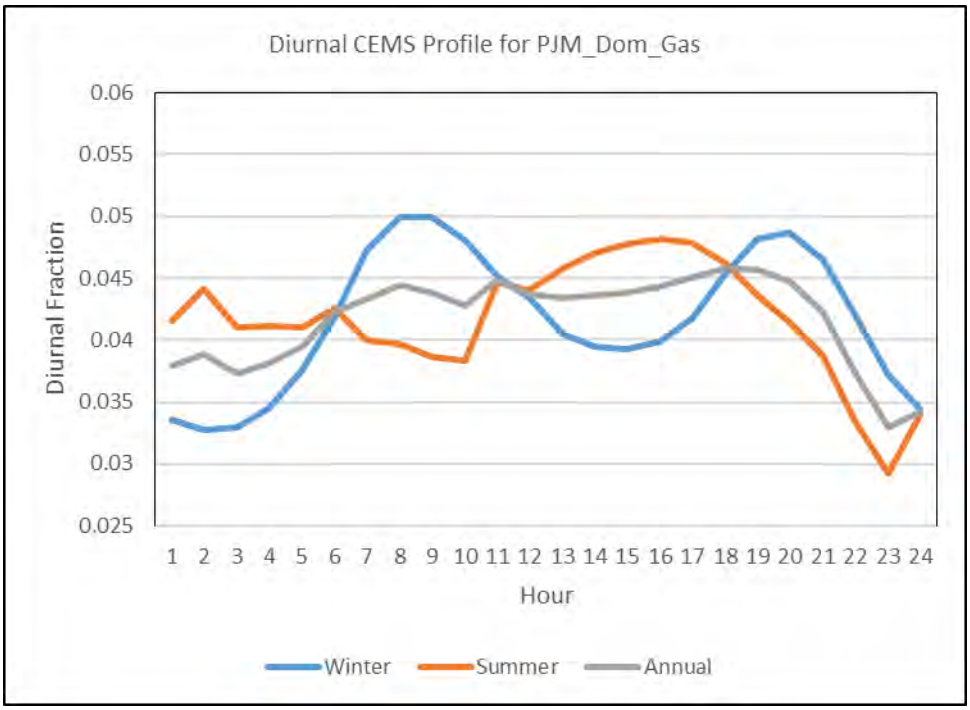


**Figure 3-5.** Seasonal diurnal profiles for EGU emissions in a Virginia Region

For sources not matched to CEMS units, temporal profiles are calculated that are used by SMOKE to allocate the annual emissions to hourly values. For these units, the allocation of the inventory annual

emissions to months is done using average fuel-specific annual-to-month factors generated for each of the 64 IPM regions shown in in Figure 3-6. These factors are based on 2014 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 other 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 2014 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 allocate $NO_X$ and $SO_2$ emissions, while CEMS heat input data are used to allocate all other pollutants. An example of month-to-day profiles for gas, coal, and an overall composite for a region in western Texas is shown in Figure 3-7.

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., 2014 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 day of the year.

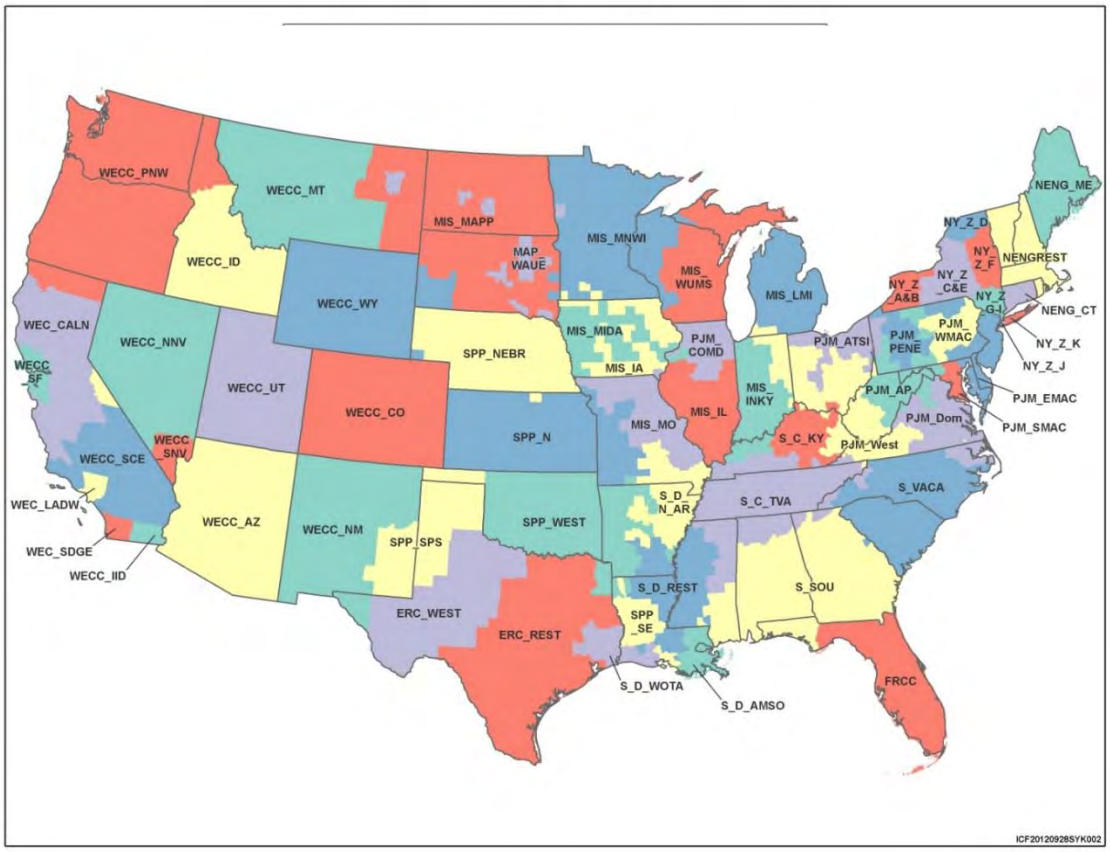


**Figure 3-6. IPM Regions for EPA Base Case v5.13**

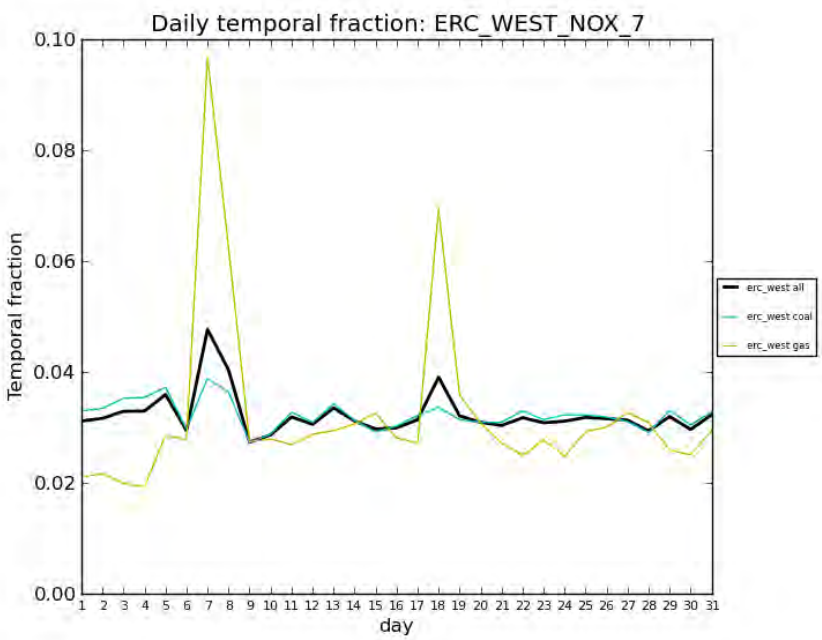


**Figure 3-7.** Month-to-day profiles for different fuels in a West Texas Region

#### *3.3.5.3 Meteorological-based Temporal Profiles*

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 method for temporalization 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 temporalization.

The SMOKE program GenTPRO provides a method for developing meteorology-based temporalization. Currently, the program can utilize three types of temporal algorithms: annual-to-day temporalization for residential wood combustion (RWC), month-to-hour temporalization for agricultural livestock ammonia, and a generic meteorology-based algorithm for other situations. For the 2014 platform, meteorological-based temporalization was used for portions of the rwc sector and for livestock within the 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 http://www.cmascenter.org/smoke/documentation/3.5.1/html/ch05s03s07.html, respectively.

As of the 2011v6.2 platform and in SMOKE 3.6.5, the temporal profile format was updated to support more flexibility in profile application. The corresponding version of GenTPRO produces separate files including the monthly temporal profiles (ATPRO_MONTHLY) and day-of-month temporal profiles (ATPRO_DAILY), instead of a single ATPRO_DAILY with day-of-year temporal profiles as it did in SMOKE 3.5. The new and old temporal allocation results are equivalent when given the same inputs.

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 3-8 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.

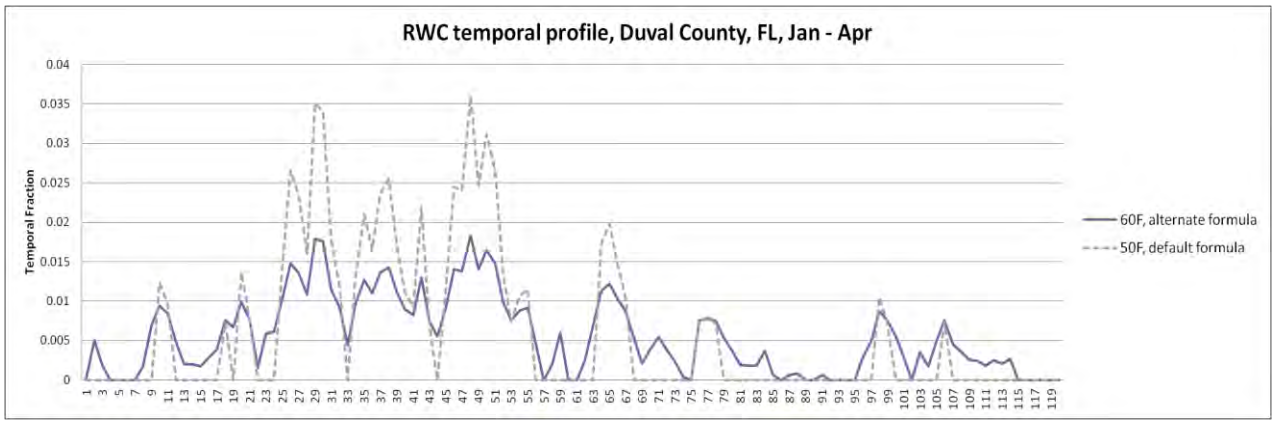


**Figure 3-8.** Example of RWC temporalization in 2007 using a 50 versus 60 ˚F threshold

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

The temporalization 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) were updated because the meteorological-based temporalization 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 (NYSERDA) "Environmental, Energy Market, and Health Characterization of Wood-Fired Hydronic Heater Technologies, Final Report" (NYSERDA, 2012) as well as a Northeast States for Coordinated Air Use Management (NESCAUM) report "Assessment of Outdoor Wood-fired Boilers" (NESCAUM, 2006). A Minnesota 2008 Residential Fuelwood Assessment Survey of individual household responses (MDNR, 2008) provided additional annual-to-month, day-of-week and diurnal activity information for OHH as well as recreational RWC usage.

The diurnal profile for OHH, shown in Figure 3-9 is based on a conventional single-stage heat load unit burning red oak in Syracuse, New York. 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 temporalization for OHH as well as recreational RWC were computed from the MN DNR survey (MDNR, 2008) and are illustrated in Figure 3-10. 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.

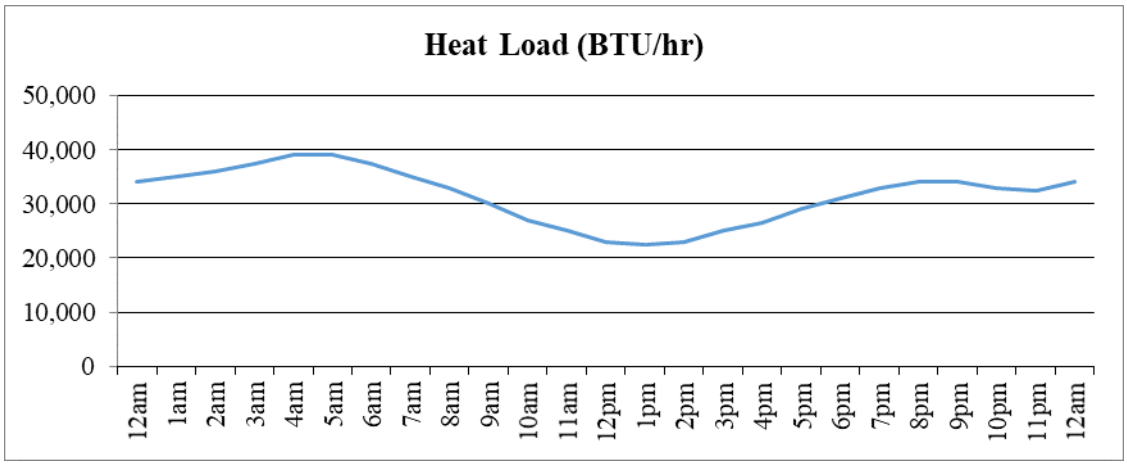


**Figure 3-9.** Diurnal profile for OHH, based on heat load (BTU/hr)

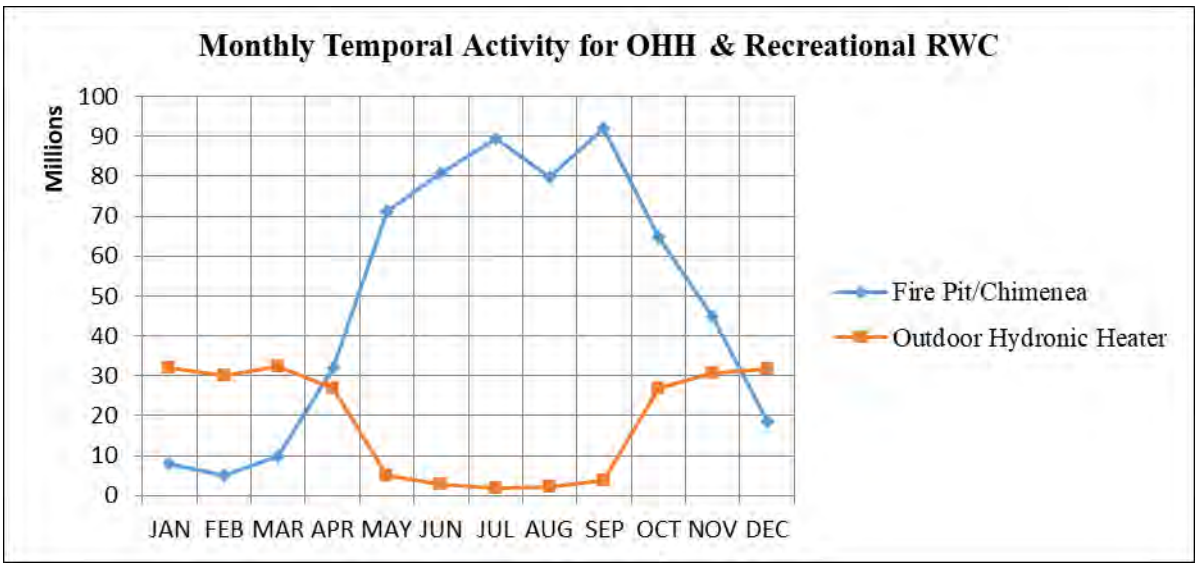


**Figure 3-10.** Annual-to-month temporal profiles for OHH and recreational RWC

For the agricultural livestock $NH_3$ algorithm, the GenTPRO algorithm is based on an equation derived by Jesse Bash of EPA ORD based on the Zhu, Henze, et al. (2014) empirical equation. This equation is based on observations from the TES satellite instrument with the GEOS-Chem model and its adjoint to estimate diurnal NH3 emission variations from livestock as a function of ambient temperature, aerodynamic resistance, and wind speed. The equations are:

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

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

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 3-11 compares the daily emissions for Minnesota from the "old" approach (uniform monthly profile) with the "new" approach (GenTPRO generated month-to-hour profiles). Although the GenTPRO profiles show daily (and hourly variability), the monthly total emissions are the same between the two approaches.

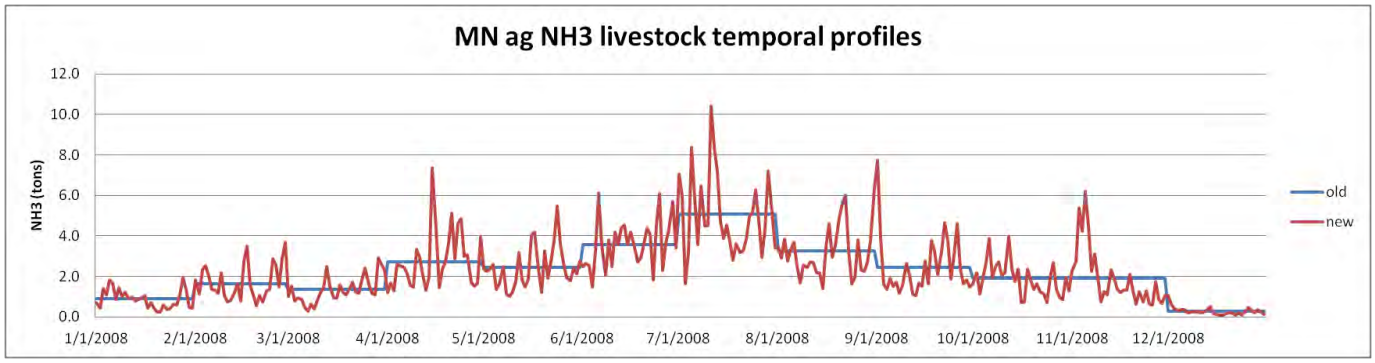


**Figure 3-11. Example of animal $NH_3$ emissions temporalization approaches, summed to daily emissions**

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, and in "Fugitive Dust Modeling for the 2008 Emissions Modeling Platform" (Adelman, 2012). The precipitation adjustment is applied to remove all emissions for days where measureable rain occurs. Therefore, the afdust emissions vary day-to-day based on the precipitation and/or snow cover for that grid cell and day. 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. 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.

### *3.3.5.4 Temporal Profiles for Onroad Mobile Sources*

For the onroad sector, the temporal distribution of emissions is a combination of more traditional temporal profiles and the influence of meteorology. This section discusses both the meteorological influences and the updates to the diurnal temporal profiles for the 2014 platform.

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) directly. Movesmrg determines the temperature for each hour and grid cell and uses that information to select the appropriate emission factor (EF) for the specified SCC/pollutant/mode combination. In the 2014 platform (and the 2014NEIv1), RPP was updated to use the gridded minimum and maximum temperature for the day. This more spatially resolved temperature range produces more accurate emissions for each grid cell. The combination of these four processes (RPD, RPV, RPH, and RPP) is the total onroad sector emissions. The onroad sector show a strong meteorological influence on their temporal patterns (see the 2014NEIv1 TSD for more details).

Figure 3-12 illustrates the difference between temporalization of the onroad sector and the meteorological influence via SMOKE-MOVES. Similar temporalization is done for the VMT in SMOKE-MOVES, but the meteorologically varying emission factors add variation on top of the temporalization.

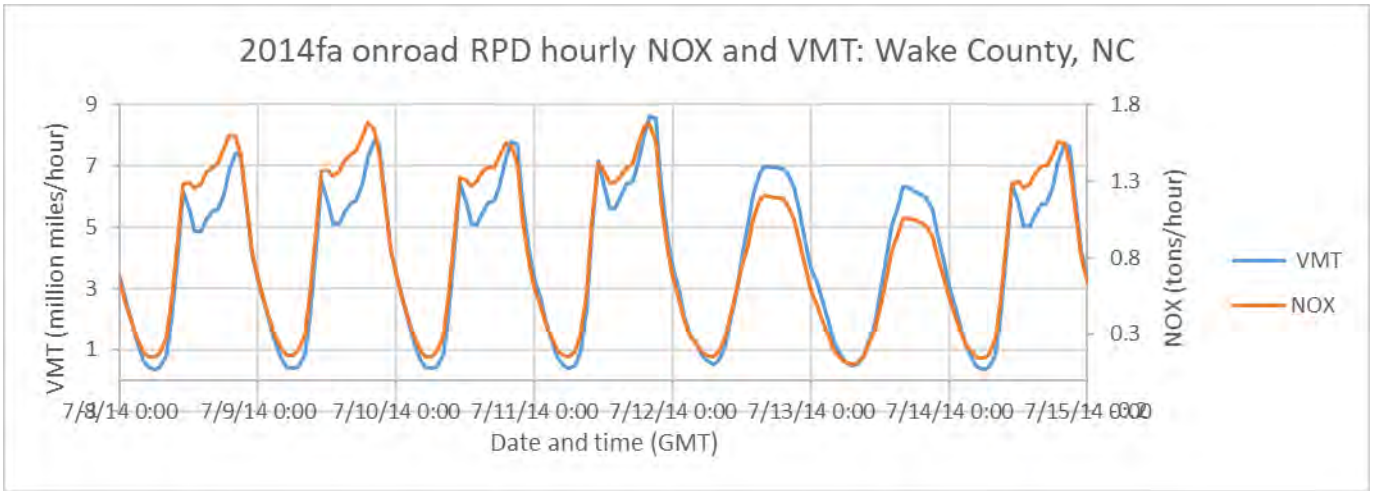


**Figure 3-12. Example of SMOKE-MOVES temporal variability of $NO_X$ emissions versus activity**

For the onroad sector, the "inventories" referred to in Table 3-11 actually consist of activity data, not emissions. For RPP and RPV processes, the VPOP inventory is annual and does not need temporalization. For RPD, the VMT inventory 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. Unlike other sectors, 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 from 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 temporalization of VMT changes. For RPH, the HOTELING inventory is annual and was temporalized to month, day of the week, and hour of the day through temporal profiles. This is an analogous process to RPD except that speed is not included in the calculation of RPH.

In previous platforms, the diurnal profile for VMT varied by road type but not by vehicle type and these profiles were used throughout the nation. Diurnal profiles that could differentiate by vehicle type as well

as by road type and would potentially vary over geography were desired. In the development of the 2011v6.0 platform, the EPA updated these profiles to include information submitted by states in their MOVES county databases (CDBs). The development of the 2014NEIv1 provided an opportunity to update these diurnal profiles with information submitted by states, to supplement the data with additional sources, and to refine the methodology.

States submitted MOVES county databases (CDBs) that included information on the distribution of VMT by hour of day and by day of week[12] (see the 2011NEIv2 TSD for details on the submittal process for onroad). The EPA mined the state submitted MOVES CDBs for non-default diurnal profiles[13]. The list of potential diurnal profiles was then analyzed to see whether the profiles varied by vehicle type, road type, weekday versus weekend, and by county within a state. For the MOVES diurnal profiles, the EPA only considered the state profiles that varied significantly by both vehicle and road types. Only those profiles that passed these criteria were used in that state or used in developing default temporal profiles. The Vehicle Travel Information System (VTRIS) is a repository for reported traffic count data to the Federal Highway Administration (FHWA). The EPA used 2012 VTRIS data to create additional temporal profiles for states that did not submit temporal information in their CDBs or where those profiles did not pass the variance criteria. The VTRIS data were used to create state specific diurnal profiles by HPMS vehicle and road type. The EPA created distinct diurnal profiles for weekdays, Saturday and Sunday along with day of the week profiles[14]. In comparison to the temporal profiles from the 2011 emissions modeling platform, the profiles for the 2014 platform include the same 2012 VTRIS data, but updated data from MOVES CDBs for 2014.

The EPA attempted to maximize the use of state and/or county specific diurnal profiles (either from MOVES or VTRIS). Where there were no MOVES or VTRIS data, then a new default profile would be used (see below for description of new profiles). This analysis was done separately for weekdays and for weekends and, therefore, some areas had submitted profiles for weekdays but defaults for weekends. The result was a set of profiles that varied geographically depending on the source of the profile and the characteristics of the profiles (see Figure 3-13).

12 The MOVES tables are the hourvmtfraction and the dayvmtfraction.

13 Further QA was done to remove duplicates and profiles that were missing two or more hours. If they were missing a single hour, the missing hour could be calculated by subtracting all other hours fractions from 1.

14 Note, the day of the week profiles (i.e., Monday vs Tuesday vs etc) are only from the VTRIS data. The MOVES CDBs only have weekday versus weekend profiles so they were not included in calculating a new national default day of the week profile.

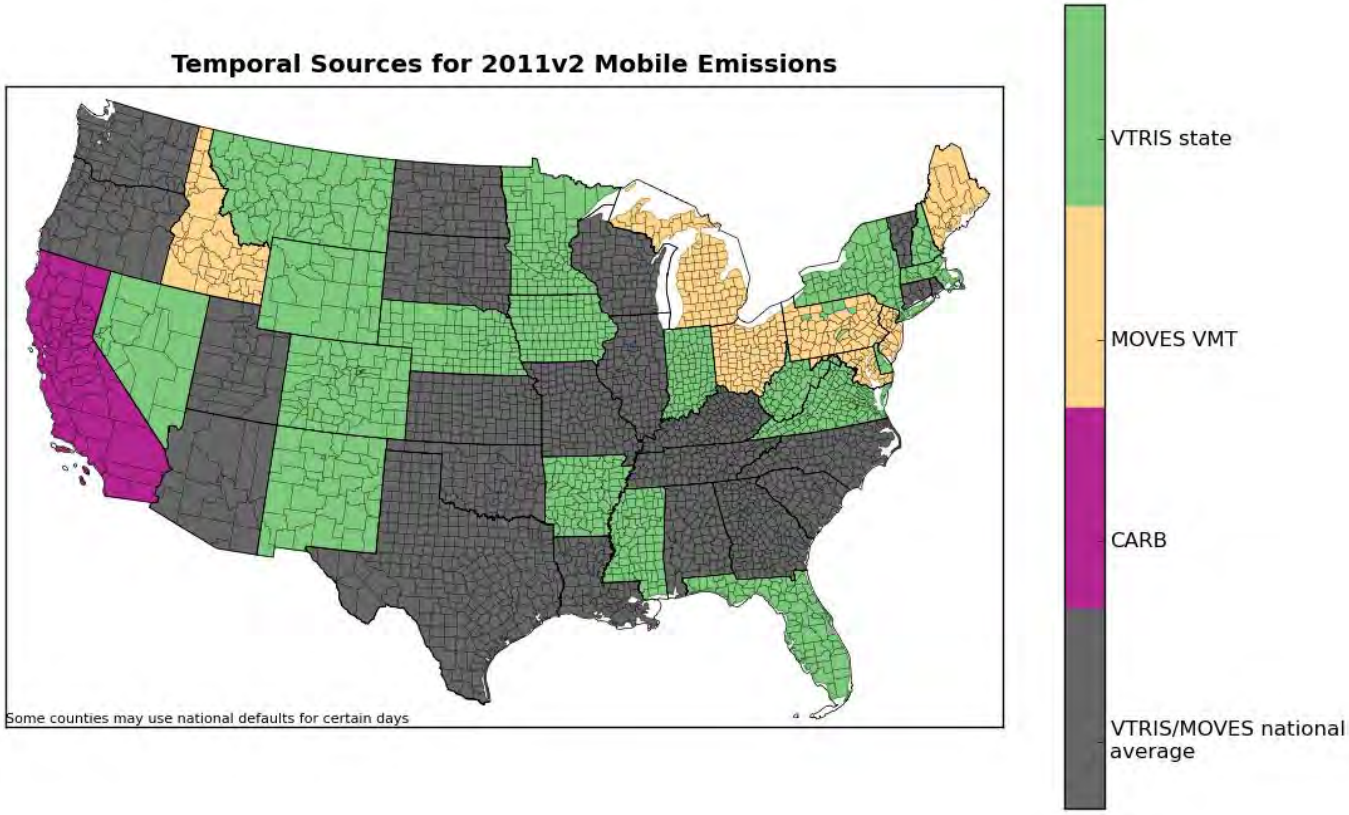


**Figure 3-13.** Use of submitted versus new national default profiles

A new set of diurnal profiles was developed from the submitted profiles that varied by both vehicle type and road type. For the purposes of constructing the national default diurnal profiles, EPA created individual profiles for each state (averaging over the counties within) to create a single profile by state, vehicle type, road type, and the day (i.e. weekday vs Saturday vs Sunday). The source of the underlying profiles was either MOVES or VTRIS data. The states individual profiles were averaged together to create a new default profile. Figure 3-14 shows two new national default profiles for light duty gas vehicles (LDGV, SCC6 220121) and combination long-haul diesel trucks (HHDDV, SCC6 220262) on restricted urban roadways (interstates and freeways). The blue lines indicate the weekday profile, the green the Saturday profile, and the red the Sunday profile. In comparison, the new default profiles for weekdays places more LDGV VMT (upper plot) in the rush hours while placing HHDDV VMT (lower plot) predominately in the middle of the day with a longer tail into the evening hours and early morning. In addition to creating diurnal profiles,

EPA also developed day of week profiles using the VTRIS data. The creation of the state and national profiles was similar to that of the diurnal profiles (described above). Figure 3-15 shows a set of national default profiles for rural restricted roads (top plot) and urban unrestricted roads (lower plot). Each vehicle type is a different color on the plots.

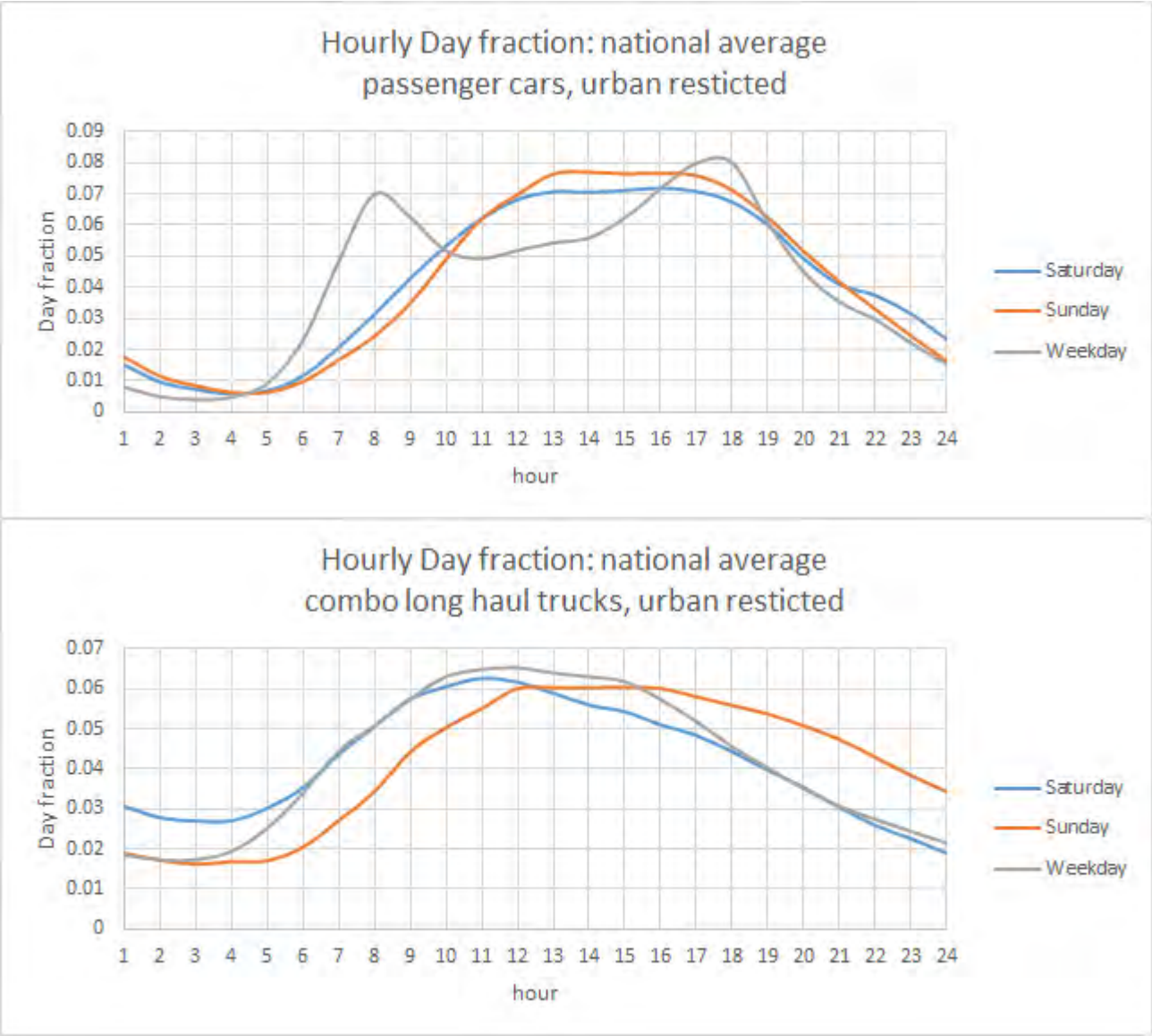


**Figure 314.** Updated national default profiles for LDGV vs. HHDDV, urban restricted

The gray lines of Figure 3-14 indicate the weekday profile, the blue the Saturday profile, and the orange the Sunday profile. In comparison, the new default profiles for weekdays places more LDGV VMT (upper plot) in the rush hours while placing HHDDV VMT (lower plot) predominately in the middle of the day with a longer tail into the evening hours and early morning. In addition to creating diurnal profiles, the EPA developed day of week profiles using the VTRIS data. The creation of the state and national profiles was similar to the diurnal profiles (described above). Figure 3-15 shows a set of national default profiles for rural restricted roads (top plot) and urban unrestricted roads (lower plot). Each vehicle type is a different color on the plots.

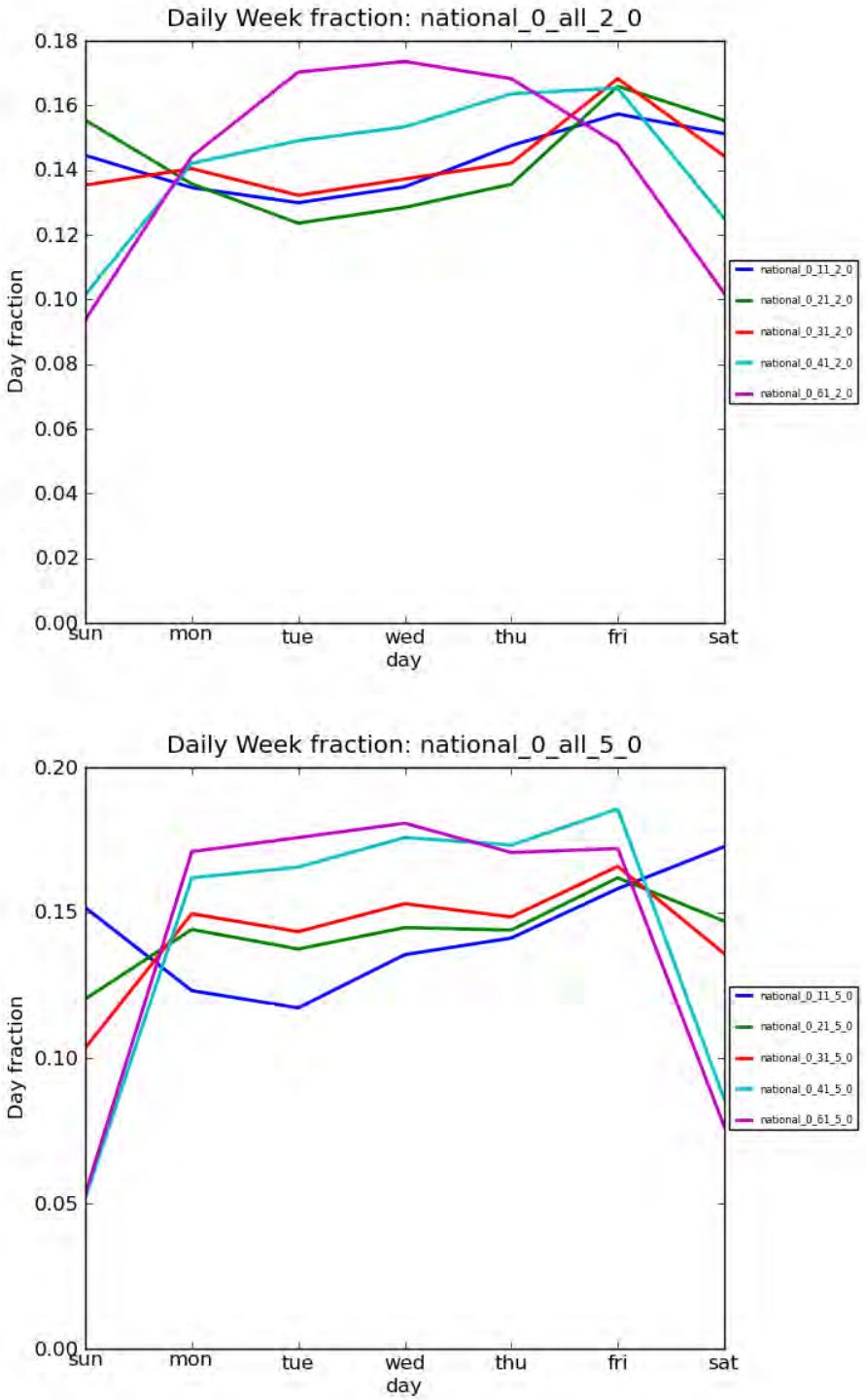


**Figure 3-15.** Updated national default profiles for day of week (top: rural restricted and bottom: urban restricted)

The EPA also developed a national profile for hoteling by averaging all the combination long-haul truck profiles on restricted roads (urban and rural) for weekdays to create a single national restricted profile (orange line in Figure 3-16). This was then inverted to create a profile for hoteling (blue line in Figure 3-16). This single national profile was used for hoteling irrespective of location.

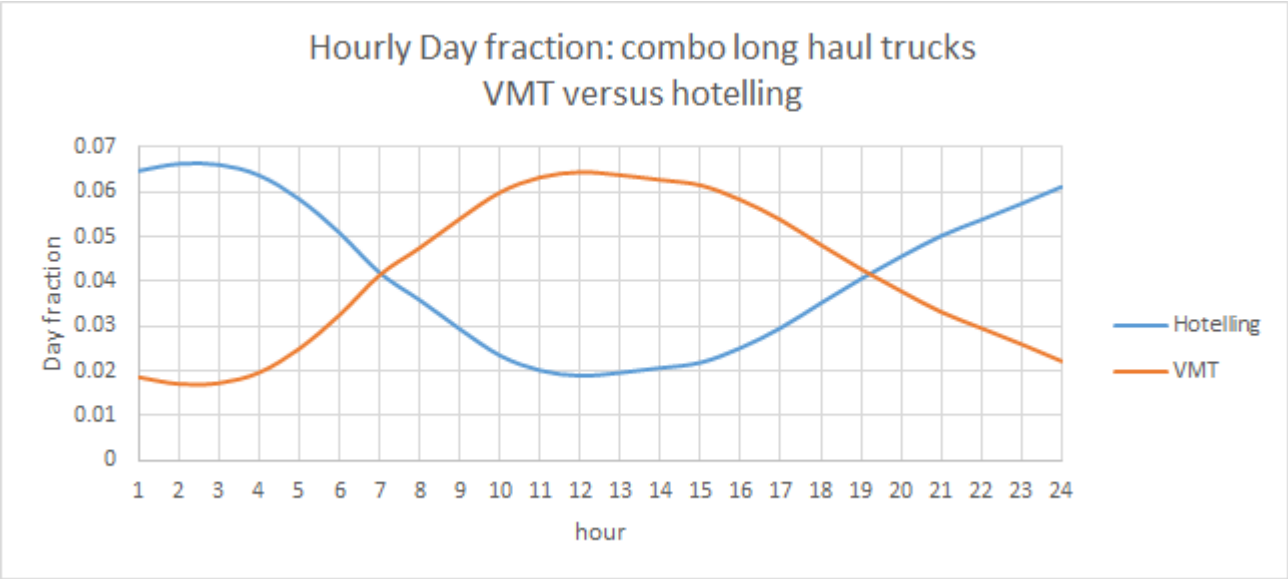


**Figure 3-16**. Combination long-haul truck restricted and hoteling profile

For California, CARB supplied diurnal profiles that varied by vehicle type, day of the week[15], and air basin. These CARB-specific profiles were used in developing EPA estimates for California. Although the EPA adjusted the total emissions to match California's submittal to the 2014NEIv1, the temporalization of these emissions took into account both the state-specific VMT profiles and the SMOKE-MOVES process of incorporating meteorology. For more details on the adjustments to California's onroad emissions, see the 2014v7.0 TSD.

### *3.3.6 Vertical Allocation of Emissions*

Table 3-5 specifies the sectors for which plume rise is calculated. If there is no plume rise for a sector, the emissions are placed into layer 1 of the air quality model. Vertical plume rise was performed in-line within CMAQ for all of the SMOKE point-source sectors (i.e., ptegu, ptnonipm, ptfire, ptagfire, othpt, and cmv_c3). The in-line plume rise computed within CMAQ is nearly identical to the plume rise that would be calculated within SMOKE using the Laypoint program. The selection of point sources for plume rise is pre-determined in SMOKE using the Elevpoint program. The calculation is done in conjunction with the CMAQ model time steps with interpolated meteorological data and is therefore more temporally resolved than when it is done in SMOKE. Also, the calculation of the location of the point sources is slightly different than the one used in SMOKE and this can result in slightly different placement of point sources near grid cell boundaries.

For point sources, the stack parameters are used as inputs to the Briggs algorithm, but point fires do not have stack parameters. However, the ptfire inventory does contain data on the acres burned (acres per day)

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

and fuel consumption (tons fuel per acre) for each day. CMAQ uses these additional parameters to estimate the plume rise of emissions into layers above the surface model layer. Specifically, these data are used to calculate heat flux, which is then used to estimate plume rise. In addition to the acres burned and fuel consumption, heat content of the fuel is needed to compute heat flux. The heat content was assumed to be 8000 Btu/lb of fuel for all fires because specific data on the fuels were unavailable in the inventory. The plume rise algorithm applied to the fires is a modification of the Briggs algorithm with a stack height of zero.

CMAQ uses the Briggs algorithm to determine the plume top and bottom, and then computes the plumes' distributions into the vertical layers that the plumes intersect. The pressure difference across each layer divided by the pressure difference across the entire plume is used as a weighting factor to assign the emissions to layers. This approach gives plume fractions by layer and source.

### *3.3.7 Emissions Modeling 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. Spatial allocation was performed for a national 12-km domain. To accomplish this, SMOKE used national 12-km spatial surrogates and a SMOKE area-to-point data file. For the U.S., EPA updated surrogates to use circa 2010-2014 data wherever possible. For Mexico, updated spatial surrogates were used as described below. For Canada, shapefiles for generating new surrogates were provided by Environment Canada for use with their 2013 inventories. The U.S., Mexican, and Canadian 12-km surrogates cover the entire CONUS domain 12US1 shown in Figure 3-2.

#### *3.3.7.1 Surrogates for U.S. Emissions*

There are more than 100 spatial surrogates available for spatially allocating U.S. county-level emissions to the 12-km grid cells used by the air quality model. Note that an area-to-point approach overrides the use of surrogates for a limited set of sources. Table 3-12 lists the codes and descriptions of the surrogates. Surrogate names and codes listed in *italics* are not directly assigned to any sources for the 2014v7.0 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 the reference Adelman, 2016.

Similar to 2011, the Surrogates for ports (801) and shipping lanes (802) were developed based on the shapes in the NEI; however they were updated using 2014NEIv1 shapefiles and activity data. The creation of surrogates and shapefiles for the U.S. was generated via the Surrogate Tool. The tool and documentation for it is available at https://www.cmascenter.org/sa-tools/documentation/4.2/SurrogateToolUserGuide_4_2.pdf.

## Table 3-12. U.S. Surrogates available for the 2014 modeling platform

| Code | Surrogate Description | Code | Surrogate Description |
|---|---|---|---|
| N/A | Area-to-point approach (see 3.3.1.2) | 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 |
| 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 |

| Code | Surrogate Description | Code | Surrogate Description |
|---|---|---|---|
| 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 | 802 | Shipping Lanes |
| *318* | *NLCD Pasture Land* | *805* | *Offshore Shipping Area* |
| 319 | NLCD Crop Land | *806* | *Offshore Shipping NEI2014 Activity* |
| 320 | NLCD Forest Land | *807* | *Navigable Waterway Miles* |
| 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 3-13. Extended (i.e., overnight) idling of trucks were assigned to surrogate 205 that is based on locations of overnight truck parking spaces. The underlying data in this surrogate was updated for use in the 2014v7.0 platform to include additional data sources and corrections based on comments received.

**Table 3-13.** 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 3-14 using 2014 data consistent with what was used to develop the 2014NEI nonpoint oil and gas emissions. The primary activity data source used for the development of the oil and gas spatial surrogates was data from Drilling Info (DI) Desktop's HPDI database (Drilling Info, 2015). This database contains well-level location, production, and exploration statistics at the monthly level. Due to a proprietary agreement with DI Desktop, individual well locations and ancillary production cannot be made publicly available, but aggregated statistics are allowed. These data were supplemented with data from state Oil and Gas Commission (OGC) websites (Illinois, Idaho, Indiana,

Kentucky, Missouri, Nevada, Oregon and Pennsylvania, Tennessee). In many cases, the correct surrogate parameter was not available (e.g., feet drilled), but an alternative surrogate parameter was available (e.g., number of spudded wells) and downloaded. Under that methodology, both completion date and date of first production from HPDI were used to identify wells completed during 2011. In total, over 1.43 million unique wells were compiled from the above data sources. The wells cover 34 states and 1,158 counties. (ERG, 2016b).

**Table 3-14. 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 3-12. U.S. Surrogates available for the 2014 modeling platform 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. The U.S. CAP emissions allocated to the various spatial surrogates are shown in Table 3-15.

**Table 315.** Selected 2014 CAP emissions by sector for U.S. Surrogates (CONUS domain totals)

| Sector | ID | Description | NH3 | NOX | PM2_5 | SO2 | VOC |
|---|---|---|---|---|---|---|---|
| afdust | 240 | Total Road Miles | | | 253,093 | | |
| afdust | 304 | NLCD Open + Low | | | 1,116,883 | | |
| afdust | 306 | NLCD Med + High | | | 45,958 | | |
| afdust | 308 | NLCD Low + Med + High | | | 139,554 | | |
| afdust | 310 | NLCD Total Agriculture | | | 1,169,400 | | |
| ag | 310 | NLCD Total Agriculture | 2,867,904 | | | | |
| cmv_c1c2 | 801 | Port Areas | 11 | 24,413 | 759 | 1,492 | 987 |
| cmv_c1c2 | 802 | Shipping Lanes | 281 | 484,726 | 13,842 | 4,129 | 8,725 |
| nonpt | 100 | Population | 32,222 | 0 | 0 | 0 | 1,137,409 |
| nonpt | 150 | Residential Heating - Natural Gas | 47,296 | 219,671 | 3,593 | 1,445 | 13,311 |
| nonpt | 170 | Residential Heating - Distillate Oil | 1,726 | 34,923 | 3,680 | 64,628 | 1,153 |
| nonpt | 180 | Residential Heating - Coal | 20 | 101 | 53 | 1,086 | 111 |
| nonpt | 190 | Residential Heating - LP Gas | 121 | 34,025 | 175 | 675 | 1,321 |
| nonpt | 239 | Total Road AADT | 0 | 25 | 552 | 0 | 276,354 |
| nonpt | 240 | Total Road Miles | 0 | 0 | 0 | 0 | 36,941 |
| nonpt | 242 | All Restricted AADT | 0 | 0 | 0 | 0 | 5,451 |
| nonpt | 244 | All Unrestricted AADT | 0 | 0 | 0 | 0 | 95,327 |
| nonpt | 271 | NTAD Class 1 2 3 Railroad Density | 0 | 0 | 0 | 0 | 2,252 |
| nonpt | 300 | NLCD Low Intensity Development | 5,183 | 24,399 | 107,748 | 2,982 | 76,167 |
| nonpt | 304 | NLCD Open + Low | 0 | 0 | 0 | 0 | 0 |
| nonpt | 306 | NLCD Med + High | 22,268 | 239,863 | 290,187 | 181,982 | 864,662 |
| nonpt | 307 | NLCD All Development | 24 | 53,320 | 144,940 | 16,485 | 611,569 |
| nonpt | 308 | NLCD Low + Med + High | 1,205 | 187,485 | 17,977 | 31,506 | 72,126 |
| nonpt | 310 | NLCD Total Agriculture | 0 | 0 | 37 | 0 | 242,713 |
| nonpt | 319 | NLCD Crop Land | 0 | 0 | 95 | 71 | 293 |
| nonpt | 320 | NLCD Forest Land | 3,984 | 13 | 54 | 0 | 61 |
| nonpt | 505 | Industrial Land | 0 | 0 | 0 | 0 | 174 |
| nonpt | 535 | Residential + Commercial + Industrial + Institutional + Government | 0 | 2 | 130 | 0 | 39 |
| nonpt | 560 | Hospital (COM6) | 0 | 0 | 0 | 0 | 0 |
| nonpt | 650 | Refineries and Tank Farms | 0 | 22 | 0 | 0 | 101,206 |
| nonpt | 711 | Airport Areas | 0 | 0 | 0 | 0 | 277 |
| nonpt | 801 | Port Areas | 0 | 0 | 0 | 0 | 7,862 |
| nonroad | 261 | NTAD Total Railroad Density | 3 | 2,593 | 273 | 4 | 503 |
| nonroad | 304 | NLCD Open + Low | 4 | 2,205 | 191 | 6 | 3,245 |
| nonroad | 305 | NLCD Low + Med | 110 | 23,017 | 4,557 | 146 | 149,863 |
| nonroad | 306 | NLCD Med + High | 345 | 243,170 | 15,750 | 526 | 126,354 |
| nonroad | 307 | NLCD All Development | 101 | 36,090 | 15,361 | 132 | 169,762 |
| nonroad | 308 | NLCD Low + Med + High | 673 | 458,488 | 38,060 | 886 | 69,386 |
| nonroad | 309 | NLCD Open + Low + Med | 111 | 22,350 | 1,257 | 148 | 44,500 |
| nonroad | 310 | NLCD Total Agriculture | 479 | 419,553 | 31,921 | 667 | 48,098 |

| Sector | ID | Description | NH3 | NOX | PM2_5 | SO2 | VOC |
|---|---|---|---|---|---|---|---|
| nonroad | 320 | NLCD Forest Land | 19 | 8,900 | 1,377 | 25 | 8,628 |
| nonroad | 321 | NLCD Recreational Land | 157 | 20,841 | 15,119 | 229 | 553,747 |
| nonroad | 350 | NLCD Water | 215 | 144,088 | 8,855 | 361 | 448,425 |
| nonroad | 693 | Well Count - All Wells | 10 | 5,845 | 229 | 12 | 1,566 |
| nonroad | 850 | Golf Courses | 13 | 2,176 | 115 | 17 | 5,668 |
| nonroad | 860 | Mines | 2 | 2,760 | 298 | 4 | 549 |
| np_oilgas | 670 | Spud Count - CBM Wells | 0 | 0 | 0 | 0 | 267 |
| np_oilgas | 671 | Spud Count - Gas Wells | 0 | 0 | 0 | 0 | 10,989 |
| np_oilgas | 672 | Gas Production at Oil Wells | 0 | 2,863 | 0 | 21,709 | 127,494 |
| np_oilgas | 673 | Oil Production at CBM Wells | 0 | 35 | 0 | 0 | 1,795 |
| np_oilgas | 674 | Unconventional Well Completion Counts | 0 | 47,606 | 1,823 | 47 | 3,150 |
| np_oilgas | 678 | Completions at Gas Wells | 0 | 3,735 | 26 | 6,328 | 74,408 |
| np_oilgas | 679 | Completions at CBM Wells | 0 | 16 | 0 | 601 | 2,155 |
| np_oilgas | 681 | Spud Count - Oil Wells | 0 | 0 | 0 | 0 | 66,565 |
| np_oilgas | 683 | Produced Water at All Wells | 0 | 10 | 0 | 0 | 67,101 |
| np_oilgas | 685 | Completions at Oil Wells | 0 | 3,107 | 130 | 2,181 | 50,785 |
| np_oilgas | 687 | Feet Drilled at All Wells | 0 | 109,487 | 4,004 | 628 | 8,130 |
| np_oilgas | 691 | Well Counts - CBM Wells | 0 | 38,117 | 603 | 15 | 34,187 |
| np_oilgas | 692 | Spud Count - All Wells | 0 | 8,628 | 258 | 135 | 366 |
| np_oilgas | 693 | Well Count - All Wells | 0 | 0 | 0 | 0 | 166 |
| np_oilgas | 694 | Oil Production at Oil Wells | 0 | 4,375 | 0 | 5,468 | 1,104,120 |
| np_oilgas | 695 | Well Count - Oil Wells | 0 | 122,856 | 3,091 | 63 | 455,552 |
| np_oilgas | 696 | Gas Production at Gas Wells | 0 | 59,634 | 3,131 | 251 | 112,335 |
| np_oilgas | 697 | Oil Production at Gas Wells | 0 | 1,360 | 0 | 26 | 354,406 |
| np_oilgas | 698 | Well Count - Gas Wells | 15 | 388,677 | 6,726 | 310 | 623,925 |
| np_oilgas | 699 | Gas Production at CBM Wells | 0 | 3,094 | 403 | 32 | 6,578 |
| onroad | 202 | Urban Restricted AADT | 24,687 | 790,075 | 30,439 | 5,846 | 149,645 |
| onroad | 205 | Extended Idle Locations | 748 | 273,106 | 4,425 | 104 | 56,079 |
| onroad | 212 | Rural Restricted AADT | 10,867 | 684,006 | 20,322 | 2,853 | 77,075 |
| onroad | 222 | Urban Unrestricted AADT | 42,001 | 1,223,593 | 54,345 | 11,950 | 376,209 |
| onroad | 232 | Rural Unrestricted AADT | 25,027 | 987,683 | 33,882 | 6,434 | 201,764 |
| onroad | 239 | Total Road AADT | | | | | 6,573 |
| onroad | 242 | All Restricted AADT | | | | | 315 |
| onroad | 258 | Intercity Bus Terminals | | 165 | 2 | 0 | 38 |
| onroad | 259 | Transit Bus Terminals | | 58 | 5 | 0 | 171 |
| onroad | 304 | NLCD Open + Low | | 821 | 22 | 1 | 2,683 |
| onroad | 306 | NLCD Med + High | | 18,500 | 384 | 20 | 22,396 |
| onroad | 307 | NLCD All Development | | 560,112 | 12,560 | 1,001 | 1,142,592 |
| onroad | 308 | NLCD Low + Med + High | | 83,977 | 1,583 | 113 | 133,883 |
| onroad | 506 | Education | | 664 | 29 | 1 | 1,107 |
| rail | 261 | NTAD Total Railroad Density | 2 | 12,494 | 297 | 282 | 736 |
| rail | 271 | NTAD Class 1 2 3 Railroad Density | 362 | 767,307 | 22,868 | 6,704 | 39,121 |

| Sector | ID | Description | NH3 | NOX | PM2_5 | SO2 | VOC |
|---|---|---|---|---|---|---|---|
| rwc | 300 | NLCD Low Intensity Development | 16,221 | 32,174 | 332,700 | 8,087 | 351,696 |

### *3.3.7.2 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, 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: https://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.

### *3.3.7.3 Surrogates for Canada and Mexico Emission Inventories*

The surrogates for Canada to spatially allocate the Canadian emissions have been updated in the platform used for this study based on the 2013 Canadian inventories and associated data. The spatial surrogate data came from Environment Canada, along with cross references. The shapefiles they provided were used in the Surrogate Tool (previously referenced) to create spatial surrogates. The Canadian surrogates used for this platform are listed in Table 3-16. Surrogates for Mexico are circa 1999 and 2000 and were based on data obtained from the Sistema Municpal de Bases de Datos (SIMBAD) de INEGI and the Bases de datos del Censo Economico 1999. CAPs allocated to the Mexico and Canada surrogates are shown in Table 3-17. The entries in Table 3-17 are for the othar, othafdust, onroad_can, and onroad_mex sectors.

**Table 3-16.** Canadian Spatial Surrogates

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

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

**Table 3-17.** CAPs Allocated to Mexican and Canadian Spatial Surrogates in 2014fb

| Code | Mexican or Canadian Surrogate Description | $NH_3$ | $NO_X$ | $PM_{2_5}$ | $SO_2$ | VOC |
|---|---|---|---|---|---|---|
| 10 | MEX Population | 0 | 216 | 6 | 1 | 434 |
| 12 | MEX Housing | 25,900 | 112,801 | 3,949 | 450 | 141,616 |
| 14 | MEX Residential Heating - Wood | 0 | 1,311 | 16,802 | 202 | 115,512 |
| 16 | MEX Residential Heating - Distillate Oil | 0 | 13 | 0 | 4 | 1 |
| 20 | MEX Residential Heating - LP Gas | 0 | 5,798 | 176 | 0 | 100 |
| 22 | MEX Total Road Miles | 2,660 | 359,254 | 10,047 | 5,692 | 75,042 |
| 24 | MEX Total Railroads Miles | 0 | 21,176 | 473 | 186 | 826 |
| 26 | MEX Total Agriculture | 180,582 | 136,198 | 28,813 | 6,529 | 10,917 |
| 32 | MEX Commercial Land | 0 | 74 | 1,615 | 0 | 21,898 |
| 34 | MEX Industrial Land | 4 | 1,080 | 1,944 | 0 | 119,006 |
| 36 | MEX Commercial plus Industrial Land | 0 | 2,027 | 30 | 5 | 95,300 |
| 38 | MEX Commercial plus Institutional Land | 3 | 1,753 | 81 | 4 | 54 |
| 40 | MEX Residential (RES1-4)+Comercial+Industrial+Institutional+Government | 0 | 4 | 11 | 0 | 74,853 |
| 42 | MEX Personal Repair (COM3) | 0 | 0 | 0 | 0 | 5,704 |
| 44 | MEX Airports Area | 0 | 3,112 | 88 | 402 | 1,062 |

| Code | Mexican or Canadian Surrogate Description | $NH_3$ | $NO_X$ | $PM_{2.5}$ | $SO_2$ | VOC |
|---|---|---|---|---|---|---|
| 50 | MEX Mobile sources - Border Crossing | 4 | 130 | 1 | 2 | 241 |
| 100 | CAN Population | 724 | 62 | 733 | 13 | 335 |
| 101 | CAN total dwelling | 383 | 34,234 | 2,538 | 4,126 | 143,234 |
| 106 | CAN ALL_INDUST | 0 | 0 | 11,559 | 0 | 72 |
| 113 | CAN Forestry and logging | 465 | 2,521 | 0 | 143 | 7,080 |
| 115 | CAN Agriculture and forestry activities | 51 | 609 | 2,941 | 13 | 1,709 |
| 200 | CAN Urban Primary Road Miles | 1,954 | 94,668 | 4,167 | 328 | 12,677 |
| 210 | CAN Rural Primary Road Miles | 779 | 57,206 | 2,297 | 134 | 5,457 |
| 212 | CAN Mining except oil and gas | 0 | 0 | 3,442 | 0 | 0 |
| 220 | CAN Urban Secondary Road Miles | 3,648 | 144,371 | 7,864 | 696 | 31,224 |
| 221 | CAN Total Mining | 0 | 0 | 56,438 | 0 | 0 |
| 222 | CAN Utilities | 79 | 9,371 | 54,184 | 3,299 | 197 |
| 230 | CAN Rural Secondary Road Miles | 2,024 | 99,071 | 4,275 | 353 | 14,291 |
| 240 | CAN Total Road Miles | 44 | 79,579 | 2,892 | 84 | 127,959 |
| 308 | CAN Food manufacturing | 0 | 0 | 11,099 | 0 | 5,873 |
| 321 | CAN Wood product manufacturing | 261 | 1,794 | 0 | 132 | 7,673 |
| 323 | CAN Printing and related support activities | 0 | 0 | 0 | 0 | 11,604 |
| 324 | CAN Petroleum and coal products manufacturing | 0 | 1,016 | 1,220 | 388 | 6,050 |
| 326 | CAN Plastics and rubber products manufacturing | 0 | 0 | 0 | 0 | 23,540 |
| 327 | CAN Non-metallic mineral product manufacturing | 0 | 0 | 6,628 | 0 | 0 |
| 331 | CAN Primary Metal Manufacturing | 0 | 156 | 5,504 | 52 | 73 |
| 412 | CAN Petroleum product wholesaler-distributors | 0 | 0 | 0 | 0 | 39,650 |
| 448 | CAN clothing and clothing accessories stores | 0 | 0 | 0 | 0 | 112 |
| 562 | CAN Waste management and remediation services | 217 | 1,631 | 2,268 | 2,275 | 16,066 |
| 921 | CAN Commercial Fuel Combustion | 185 | 23,982 | 2,251 | 3,760 | 1,154 |
| 923 | CAN TOTAL INSTITUTIONAL AND GOVERNEMNT | 0 | 0 | 0 | 0 | 13,707 |
| 924 | CAN Primary Industry | 0 | 0 | 0 | 0 | 35,196 |
| 925 | CAN Manufacturing and Assembly | 0 | 0 | 0 | 0 | 69,833 |
| 926 | CAN Distribtution and Retail (no petroleum) | 0 | 0 | 0 | 0 | 6,990 |
| 927 | CAN Commercial Services | 0 | 0 | 0 | 0 | 30,189 |
| 932 | CAN CANRAIL | 54 | 119,139 | 2,773 | 430 | 5,936 |
| 941 | CAN PAVED ROADS | 0 | 0 | 297,607 | 0 | 0 |
| 945 | CAN Commercial Marine Vessels | 187 | 152,803 | 5,579 | 34,596 | 11,045 |

| Code | Mexican or Canadian Surrogate Description | $NH_3$ | $NO_X$ | $PM_{2.5}$ | $SO_2$ | VOC |
|---|---|---|---|---|---|---|
| 950 | CAN Combination of Forest and Dwelling | 1,733 | 19,252 | 158,532 | 2,750 | 224,453 |
| 955 | CAN UNPAVED_ROADS_AND_TRAILS | 0 | 0 | 440,673 | 0 | 0 |
| 960 | CAN TOTBEEF | 0 | 0 | 1,236 | 0 | 263,913 |
| 965 | CAN TOTBEEF_CD | 280,058 | 0 | 0 | 0 | 0 |
| 966 | CAN TOTPOUL_CD | 23,809 | 0 | 0 | 0 | 0 |
| 967 | CAN TOTSWIN_CD | 67,992 | 0 | 0 | 0 | 0 |
| 968 | CAN TOTFERT_CD | 120,304 | 0 | 0 | 0 | 0 |
| 970 | CAN TOTPOUL | 0 | 0 | 181 | 0 | 242 |
| 980 | CAN TOTSWIN | 0 | 0 | 756 | 0 | 2,585 |
| 990 | CAN TOTFERT | 0 | 4,227 | 379,893 | 9,448 | 155 |
| 996 | CAN urban_area | 0 | 0 | 1,265 | 0 | 0 |
| 1211 | CAN Oil and Gas Extraction | 2 | 29 | 228,599 | 152 | 922 |
| 1212 | CAN OilSands | 126 | 2,053 | 0 | 638 | 1,754 |
| 1251 | CAN OFFR_TOTFERT | 109 | 118,124 | 8,753 | 79 | 10,866 |
| 1252 | CAN OFFR_MINES | 42 | 41,444 | 3,443 | 31 | 4,175 |
| 1253 | CAN OFFR Other Construction not Urban | 26 | 23,606 | 3,885 | 20 | 9,504 |
| 1254 | CAN OFFR Commercial Services | 34 | 17,807 | 2,203 | 29 | 22,700 |
| 1255 | CAN OFFR Oil Sands Mines | 0 | 0 | 0 | 0 | 0 |
| 1256 | CAN OFFR Wood industries CANVEC | 13 | 11,553 | 1,103 | 10 | 1,921 |
| 1258 | CAN OFFR_Utilities | 16 | 8,553 | 529 | 14 | 10,136 |
| 1259 | CAN OFFR total dwelling | 17 | 5,399 | 1,409 | 14 | 34,499 |
| 1260 | CAN OFFR_water | 8 | 2,050 | 302 | 11 | 18,222 |
| 1261 | CAN OFFR_ALL_INDUST | 4 | 4,171 | 267 | 3 | 860 |
| 1262 | CAN OFFR Oil and Gas Extraction | 1 | 1,036 | 57 | 1 | 148 |
| 1263 | CAN OFFR_ALLROADS | 33 | 10,427 | 1,670 | 28 | 62,496 |
| 1264 | CAN OFFR_OTHERJET | 1 | 848 | 71 | 1 | 72 |
| 1265 | CAN OFFR_CANRAIL | 0 | 85 | 8 | 0 | 14 |

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# 4.0 CMAQ Air Quality Model Estimates

## 4.1 Introduction to the CMAQ Modeling Platform

The Clean Air Act (CAA) provides a mandate to assess and manage air pollution levels to protect human health and the environment. EPA has established National Ambient Air Quality Standards (NAAQS), requiring the development of effective emissions control strategies for such pollutants as ozone and particulate matter. Air quality models are used to develop these emission control strategies to achieve the objectives of the CAA.

Historically, air quality models have addressed individual pollutant issues separately. However, many of the same precursor chemicals are involved in both ozone and aerosol (particulate matter) chemistry; therefore, the chemical transformation pathways are dependent. Thus, modeled abatement strategies of pollutant precursors, such as volatile organic compounds (VOC) and NOx to reduce ozone levels, may exacerbate other air pollutants such as particulate matter. To meet the need to address the complex relationships between pollutants, EPA developed the Community Multiscale Air Quality (CMAQ) modeling system[15.] The primary goals for CMAQ are to:

- Improve the environmental management community's ability to evaluate the impact of air quality management practices for multiple pollutants at multiple scales.
- Improve the scientist's ability to better probe, understand, and simulate chemical and physical interactions in the atmosphere.

The CMAQ modeling system brings together key physical and chemical functions associated with the dispersion and transformations of air pollution at various scales. It was designed to approach air quality as a whole by including state-of-the-science capabilities for modeling multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation. CMAQ relies on emission estimates from various sources, including the U.S. EPA Office of Air Quality Planning and Standards' current emission inventories, observed emission from major utility stacks, and model estimates of natural emissions from biogenic and agricultural sources. CMAQ also relies on meteorological predictions that include assimilation of meteorological observations as constraints. Emissions and meteorology data are fed into CMAQ and run through various algorithms that simulate the physical and chemical processes in the atmosphere to provide estimated concentrations of the pollutants. Traditionally, the model has been used to predict air quality across a regional or national domain and then to simulate the effects of various changes in emission levels for policymaking purposes. For health studies, the model can also be used to provide supplemental information about air quality in areas where no monitors exist.

CMAQ was also designed to have multi-scale capabilities so that separate models were not needed for urban and regional scale air quality modeling. The CMAQ simulation performed for this 2014 assessment used a single domain that covers the entire continental U.S. (CONUS) and large portions of Canada and

[15] Byun, D.W., and K. L. Schere, 2006: Review of the Governing Equations, Computational Algorithms, and Other Components of the Models-3 Community Multiscale Air Quality (CMAQ) Modeling System. Applied Mechanics Reviews, Volume 59, Number 2 (March 2006), pp. 51-77.

Mexico using 12 km by 12 km horizontal grid spacing. Currently, 12 km x 12 km resolution is sufficient as the highest resolution for most regional-scale air quality model applications and assessments.[16] With the temporal flexibility of the model, simulations can be performed to evaluate longer term (annual to multi-year) pollutant climatologies as well as short-term (weeks to months) transport from localized sources. By making CMAQ a modeling system that addresses multiple pollutants and different temporal and spatial scales, CMAQ has a "one atmosphere" perspective that combines the efforts of the scientific community. Improvements will be made to the CMAQ modeling system as the scientific community further develops the state-of-the-science.

For more information on CMAQ, go to https://www.epa.gov/cmaq or http://www.cmascenter.org.

### *4.1.1 Advantages and Limitations of the CMAQ Air Quality Model*

An advantage of using the CMAQ model output for characterizing air quality for use in comparing with health outcomes is that it provides a complete spatial and temporal coverage across the U.S. CMAQ is a three-dimensional Eulerian photochemical air quality model that simulates the numerous physical and chemical processes involved in the formation, transport, and destruction of ozone, particulate matter and air toxics for given input sets of initial and boundary conditions, meteorological conditions and emissions. The CMAQ model includes state-of-the-science capabilities for conducting urban to regional scale simulations of multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition and visibility degradation. However, CMAQ is resource intensive, requiring significant data inputs and computing resources.

An uncertainty of using the CMAQ model includes structural uncertainties, representation of physical and chemical processes in the model. These consist of: choice of chemical mechanism used to characterize reactions in the atmosphere, choice of land surface model and choice of planetary boundary layer. Another uncertainty in the CMAQ model is based on parametric uncertainties, which includes uncertainties in the model inputs: hourly meteorological fields, hourly 3-D gridded emissions, initial conditions, and boundary conditions. Uncertainties due to initial conditions are minimized by using a 10-day ramp-up period from which model results are not used in the aggregation and analysis of model outputs. Evaluations of models against observed pollutant concentrations build confidence that the model performs with reasonable accuracy despite the uncertainties listed above. A detailed model evaluation for ozone and $PM_{2.5}$ species provided in Section 4.3 shows generally acceptable model performance which is equivalent or better than typical state-of-the-science regional modeling simulations as summarized in Simon et al., 2012[17].

## 4.2 CMAQ Model Version, Inputs and Configuration

This section describes the air quality modeling platform used for the 2014 CMAQ simulation. A modeling platform is a structured system of connected modeling-related tools and data that provide a consistent and transparent basis for assessing the air quality response to changes in emissions and/or meteorology. A platform typically consists of a specific air quality model, emissions estimates, a set of meteorological inputs, and estimates of "boundary conditions" representing pollutant transport from source areas outside

[16] U.S. EPA (2014), Draft Modeling Guidance for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze, pp 214. https://www3.epa.gov/ttn/scram/guidance/guide/Draft_O3-PM-RH_Modeling_Guidance-2014.pdf .
[17] Simon, H., Baker, K.R., and Phillips, S. (2012) Compilation and interpretation of photochemical model performance statistics published between 2006 and 2012. *Atmospheric Environment* **61**, 124-139.

the region modeled. We used the CMAQ modeling system coupled to the Weather Research and Forecasting (WRF) meteorological model as part of the 2014 Platform to provide a national scale air quality modeling analysis. The CMAQ model simulates the multiple physical and chemical processes involved in the formation, transport, and destruction of ozone and fine particulate matter ($PM_{2.5}$).

This section provides a description of each of the main components of the 2014 CMAQ-WRF simulation along with the results of a model performance evaluation in which the 2014 model predictions are compared to corresponding measured ambient concentrations.

### *4.2.1 CMAQ Model Version*

CMAQ is a non-proprietary computer model that simulates the formation and fate of photochemical oxidants, including $PM_{2.5}$ and ozone, for given input sets of meteorological conditions and emissions. As mentioned previously, CMAQ includes numerous science modules that simulate the emission, production, decay, deposition and transport of organic and inorganic gas-phase and pollutants in the atmosphere. This 2014 analysis employed CMAQ version 5.2[18] coupled to the Weather Research and Forecasting (WRF) version 3.8.1.[19] Two-way feedback was not utilized in this 2014 simulation, however, CMAQ read WRF meteorological data on a five-minute interval. The 2014 CMAQ-WRF run included bi-directional ammonia ($NH_3$) air-surface exchange (v2.1) using the Massad formulation[20], CB6r3 chemical mechanism, AERO6 aerosol module with non-volatile Primary Organic Aerosol (POA), and windblown dust algorithms. The CMAQ community model versions 5.0.2 and 5.1 were most recently peer-reviewed in September of 2015 for the U.S. EPA.[21]

### *4.2.2 Model Domain and Grid Resolution*

The WRF-CMAQ modeling analyses were performed for a domain covering the continental United States, as shown in Figure 4-1. This single domain covers the entire continental U.S. (CONUS) and large portions of Canada and Mexico using 12 km by 12 km horizontal grid spacing. The 2014 simulation used a Lambert Conformal map projection centered at (-97, 40) with true latitudes at 33 and 45 degrees north. The 12 km WRF-CMAQ domain consisted of 459 by 299 grid cells and 35 vertical layers. Table 4-1 provides some basic geographic information regarding the 12 km WRF-CMAQ domain. The model extends vertically from the surface to 50 millibars (approximately 17,600 meters) using a sigma-pressure coordinate system. Table 4-2 shows the vertical layer structure used in the 2014 simulation. Air quality conditions at the outer boundary of the 12-km domain were taken from a global model.

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[18] CMAQ version 5.2 model code is available from the Community Modeling and Analysis System (CMAS) at: http://www.cmascenter.org.

[19] Skamarock, W.C. and J.B. Klemp, 2008. A time-split nonhydrostatic atmospheric model for weather research and forecasting applications. Journal of Computation Physics, Volume 227, pp. 3465-3485.

[20] Massad, R.-S., Nemitz, E., and Sutton, M.A. (2010). Review and parameterization of bi-directional ammonia exchange between vegetation and the atmosphere, Atmos. Chem. Phys., 10, 10359-10386, doi:10.5194/acp-10-10359-2010.

[21] Moran, M.D., Astitha, M., Barsanti, K.C., Brown, N.J., Kaduwela, A., McKeen, S.A., Pickering, K.E. (September 28, 2015). Final Report: Fifth Peer Review of the CMAQ Model, https://www.epa.gov/sites/production/files/2016-11/documents/cmaq_fifth_review_final_report_2015.pdf. This peer review was focused on CMAQ v5.0.2, which was released in May, 2014, as well as CMAQ v5.1, which was released in October 2015. It is available from the Community Modeling and Analysis System (CMAS) as well as previous peer-review reports at: http://www.cmascenter.org.

**Table 4-1. Geographic Information for 12 km Modeling Domain**

| National 12 km WRF-CMAQ Modeling Configuration | |
|---|---|
| Map Projection | Lambert Conformal Projection |
| Grid Resolution | 12 km |
| Coordinate Center | 97 W, 40 N |
| True Latitudes | 33 and 45 N |
| Dimensions | 459 x 299 x 35 |
| Vertical Extent | 35 Layers: Surface to 50 mb level (see Table 4-2) |

**Table 4-2. Vertical layer structure for 2014 WRF-CMAQ simulation (heights are layer top).**

| Vertical Layers | Sigma P | Pressure (mb) | Approximate Height (m) |
|---|---|---|---|
| 35 | 0.0000 | 50.00 | 17,556 |
| 34 | 0.0500 | 97.50 | 14,780 |
| 33 | 0.1000 | 145.00 | 12,822 |
| 32 | 0.1500 | 192.50 | 11,282 |
| 31 | 0.2000 | 240.00 | 10,002 |
| 30 | 0.2500 | 287.50 | 8,901 |
| 29 | 0.3000 | 335.00 | 7,932 |
| 28 | 0.3500 | 382.50 | 7,064 |
| 27 | 0.4000 | 430.00 | 6,275 |
| 26 | 0.4500 | 477.50 | 5,553 |
| 25 | 0.5000 | 525.00 | 4,885 |
| 24 | 0.5500 | 572.50 | 4,264 |
| 23 | 0.6000 | 620.00 | 3,683 |
| 22 | 0.6500 | 667.50 | 3,136 |
| 21 | 0.7000 | 715.00 | 2,619 |
| 20 | 0.7400 | 753.00 | 2,226 |
| 19 | 0.7700 | 781.50 | 1,941 |
| 18 | 0.8000 | 810.00 | 1,665 |
| 17 | 0.8200 | 829.00 | 1,485 |
| 16 | 0.8400 | 848.00 | 1,308 |
| 15 | 0.8600 | 867.00 | 1,134 |
| 14 | 0.8800 | 886.00 | 964 |
| 13 | 0.9000 | 905.00 | 797 |

| Vertical Layers | Sigma P | Pressure (mb) | Approximate Height (m) |
|---|---|---|---|
| 12 | 0.9100 | 914.50 | 714 |
| 11 | 0.9200 | 924.00 | 632 |
| 10 | 0.9300 | 933.50 | 551 |
| 9 | 0.9400 | 943.00 | 470 |
| 8 | 0.9500 | 952.50 | 390 |
| 7 | 0.9600 | 962.00 | 311 |
| 6 | 0.9700 | 971.50 | 232 |
| 5 | 0.9800 | 981.00 | 154 |
| 4 | 0.9850 | 985.75 | 115 |
| 3 | 0.9900 | 990.50 | 77 |
| 2 | 0.9950 | 995.25 | 38 |
| 1 | 0.9975 | 997.63 | 19 |
| 0 | 1.0000 | 1000.00 | 0 |

**Figure 4-1. Map of the 2014 WRF-CMAQ Modeling Domain. The blue box denotes the 12-km national modeling domain.**

### *4.2.3 Modeling Period / Ozone Episodes*

The 12-km WRF-CMAQ modeling domain was modeled for the entire year of 2014. The annual simulation included a "ramp-up" period, comprised of 10 days before the beginning of the simulation, to mitigate the effects of initial concentrations. All 365 model days were used in the annual average levels of $PM_{2.5}$. For the 8-hour ozone, we used modeling results from the period between May 1 and September 30. This 153-day period generally conforms to the ozone season across most parts of the U.S. and contains the majority of days that observed high ozone concentrations.

### *4.2.4 Model Inputs: Emissions, Meteorology and Boundary Conditions*

*2014 Emissions:* The emissions inventories used in the 2014 air quality modeling are described in Section 3, above.

*Meteorological Input Data:* The gridded meteorological data for the entire year of 2014 at the 12 km continental United States scale domain was derived from version 3.8.1[22] of the Weather Research and Forecasting Model (WRF), Advanced Research WRF (ARW) core.[23] The WRF Model is a state-of-the-science mesoscale numerical weather prediction system developed for both operational forecasting and atmospheric research applications (http://wrf-model.org ). The 2014 CMAQ-WRF meteorology simulated for 2014 with 2011 National Land Cover Database (NLCD)[24] and using version 2 four-dimensional data assimilation with no nudging in the planetary boundary layer and based on blended 3-hourly reanalysis fields (combination of 6-hour *(*Meteorological Assimilation Data Ingest System*)* MADIS[25] data and intermediate North American Mesoscale Model[26] (NAM) 3-hour forecast) organized into 12km NAM Data Assimilation System (NDAS) fields up to 50 hPa. The WRF simulation included the physics options of the Pleim-Xiu land surface model (LSM) with NLCD woody wetlands lad use category recognized, Asymmetric Convective Model version 2 planetary boundary layer (PBL) scheme, Morrison double moment microphysics, Kain- Fritsch cumulus parameterization scheme utilizing the moisture-advection trigger[27] and the RRTMG long-wave and shortwave radiation (LWR/SWR) scheme.[28] In addition, the Group for High Resolution Sea Surface Temperatures (GHRSST)[29,30] 1km SST data was used for SST information to provide more resolved information compared to the more coarse data in the NAM analysis.

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[22] Version 3.6.1 was the current version of WRF at the time the 2013 meteorological model simulation was performed.
[23] Skamarock, W.C., Klemp, J.B., Dudhia, J., Gill, D.O., Barker, D.M., Duda, M.G., Huang, X., Wang, W., Powers, J.G., 2008. A Description of the Advanced Research WRF Version 3.
[24] National Land Cover Database 2011, http://www.mrlc.gov/nlcd2011.php
[25] Meteorological Assimilation Data Ingest System. http://madis.noaa.gov/.
[26] North American Model Analysis-Only, http://nomads.ncdc.noaa.gov/data.php; download from ftp://nomads.ncdc.noaa.gov/NAM/analysis_only/.
[27] Ma, L-M. and Tan, Z-M, 2009. Improving the behavior of the Cumulus Parameterization for Tropical Cyclone Prediction: Convection Trigger. Atmospheric Research 92 Issue 2, 190-211. http://www.sciencedirect.com/science/article/pii/S0169809508002585
[28] Gilliam, R.C., Pleim, J.E., 2010. Performance Assessment of New Land Surface and Planetary Boundary Layer Physics in the WRF-ARW. Journal of Applied Meteorology and Climatology 49, 760-774.
[29] Stammer, D., F.J. Wentz, and C.L. Gentemann, 2003, Validation of Microwave Sea Surface Temperature Measurements for Climate Purposes, J. Climate, 16, 73-87.
[30] Global High Resolution SST (GHRSST) analysis, https://www.ghrsst.org/.

*Initial and Boundary Conditions:* The lateral boundary and initial species concentrations are provided by a three-dimensional global atmospheric chemistry model, the GEOS-CHEM[31] model version 10-1, using the tropchem, NOx_Ox_HC_Aer_Br, mechanism. The global GEOS-CHEM model simulates atmospheric chemical and physical processes driven by assimilated meteorological observations from the NASA's Goddard Earth Observing System (GEOS-5). This model was run for 2014 with a grid resolution of 2.0 degrees x 2.5 degrees (latitude-longitude). The predictions were processed using the GEOS-2-CMAQ tool and used to provide one-way dynamic boundary conditions at one-hour intervals.[32,33] More information is available about the GEOS-CHEM model and other applications using this tool at: http://gmao.gsfc.nasa.gov/GEOS/ and http://wiki.seas.harvard.edu/geos-chem/index.php/GEOS-5.

## 4.3 CMAQ Model Performance Evaluation

An operational model performance evaluation for ozone and $PM_{2.5}$ and its related speciated components was conducted for the 2014 simulation using state/local monitoring sites data in order to estimate the ability of the CMAQ modeling system to replicate the 2014 base year concentrations for the 12 km continental U.S. domain.

There are various statistical metrics available and used by the science community for model performance evaluation. For a robust evaluation, the principal evaluation statistics used to evaluate CMAQ performance were two bias metrics, mean bias and normalized mean bias; and two error metrics, mean error and normalized mean error.

Mean bias (MB) is used as average of the difference (predicted – observed) divided by the total number of replicates ($n$). Mean bias is defined as:

$$\text{MB} = \frac{1}{n}\sum_{1}^{n}(P - O)$$ , where P = predicted and O = observed concentrations.

Mean error (ME) calculates the absolute value of the difference (predicted - observed) divided by the total number of replicates ($n$). Mean error is defined as:

$$\text{ME} = \frac{1}{n}\sum_{1}^{n}|P - O|$$

Normalized mean bias (NMB) is used as a normalization to facilitate a range of concentration magnitudes. This statistic averages the difference (model - observed) over the sum of observed values. NMB is a useful model performance indicator because it avoids overinflating the observed range of values, especially at low concentrations. Normalized mean bias is defined as:

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[31] Yantosca, B., 2004. GEOS-CHEMv7-01-02 User's Guide, Atmospheric Chemistry Modeling Group, Harvard University, Cambridge, MA, October 15, 2004.

[32] Akhtar, F., Henderson, B., Appel, W., Napelenok, S., Hutzell, B., Pye, H., Foley, K., 2012. Multiyear Boundary Conditions for CMAQ 5.0 from GEOS-Chem with Secondary Organic Aerosol Extensions, 11th Annual Community Modeling and Analysis System conference, Chapel Hill, NC, October 2012.

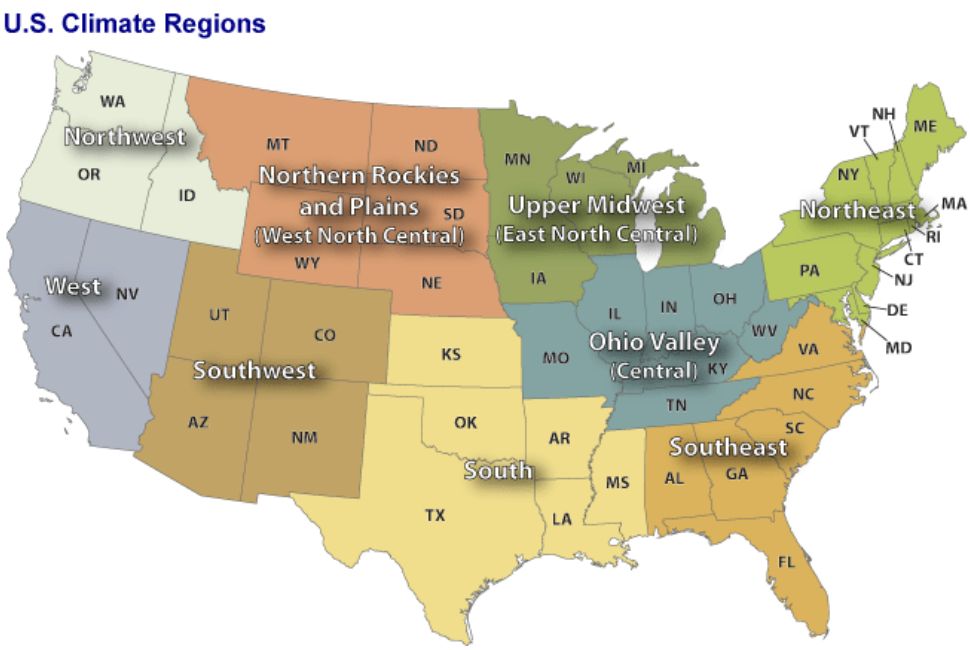
[33] Henderson, B.H., Akhtar, F., Pye, H.O.T., Napelenok, S.L., and Hutzell, W.T. (2014) A database and tool for boundary conditions for regional air quality modeling: description and evaluation, Geosci. Model Dev., **7**, 339-360.

$$\text{NMB} = \frac{\sum_{1}^{n}(P-O)}{\sum_{1}^{n}(O)} *100, \text{ where P = predicted concentrations and O = observed}$$

Normalized mean error (NME) is also similar to NMB, where the performance statistic is used as a normalization of the mean error. NME calculates the absolute value of the difference (model - observed) over the sum of observed values. Normalized mean error is defined as:

$$\text{NME} = \frac{\sum_{1}^{n}|P-O|}{\sum_{1}^{n}(O)} *100$$

The performance statistics were calculated using predicted and observed data that were paired in time and space on an 8-hour basis. Statistics were generated for each of the nine National Oceanic and Atmospheric Administration (NOAA) climate regions[34] of the 12-km U.S. modeling domain (Figure 4-2). The regions include the Northeast, Ohio Valley, Upper Midwest, Southeast, South, Southwest, Northern Rockies, Northwest and West[35,36] as were originally identified in Karl and Koss (1984)[37].




[34] NOAA, National Centers for Environmental Information scientists have identified nine climatically consistent regions within the contiguous U.S., http://www.ncdc.noaa.gov/monitoring-references/maps/us-climate-regions.php.

[35] The nine climate regions are defined by States where: Northeast includes CT, DE, ME, MA, MD, NH, NJ, NY, PA, RI, and VT; Ohio Valley includes IL, IN, KY, MO, OH, TN, and WV; Upper Midwest includes IA, MI, MN, and WI; Southeast includes AL, FL, GA, NC, SC, and VA; South includes AR, KS, LA, MS, OK, and TX; Southwest includes AZ, CO, NM, and UT; Northern Rockies includes MT, NE, ND, SD, WY; Northwest includes ID, OR, and WA; and West includes CA and NV.

[36] Note most monitoring sites in the West region are located in California (see Figure 4-2), therefore statistics for the West will be mostly representative of California ozone air quality.

[37] Karl, T. R. and Koss, W. J., 1984: "Regional and National Monthly, Seasonal, and Annual Temperature Weighted by Area, 1895-1983." Historical Climatology Series 4-3, National Climatic Data Center, Asheville, NC, 38 pp.

**Figure 4-2. NOAA Nine Climate Regions (source: http://www.ncdc.noaa.gov/monitoring-references/maps/us-climate-regions.php#references)**

In addition to the performance statistics, regional maps which show the MB, ME, NMB, and NME were prepared for the ozone season, May through September, at individual monitoring sites as well as on an annual basis for $PM_{2.5}$ and its component species.

*Evaluation for 8-hour Daily Maximum Ozone:* The operational model performance evaluation for eight-hour daily maximum ozone was conducted using the statistics defined above. Ozone measurements for 2014 in the continental U.S. were included in the evaluation and were taken from the 2014 State/local monitoring site data in the EPA Air Quality System (AQS) and the Clean Air Status and Trends Network (CASTNet).

The 8-hour ozone model performance bias and error statistics for each of the nine NOAA climate regions and each season are provided in Table 4-4. Seasons were defined as: winter (December-January-February), spring (March-April-May), summer (June, July, August), and fall (September-October-November). In some instances, observational data were excluded from the analysis and model evaluation based on a completeness criterion of 75 percent. Spatial plots of the MB, ME, NMB and NME for individual monitors are shown in Figures 4-3 through 4-6, respectively. The statistics shown in these two figures were calculated over the ozone season, May through September, using data pairs on days with observed 8-hour ozone of greater than or equal to 60 ppb.

In general, the model performance statistics indicate that the 8-hour daily maximum ozone concentrations predicted by the 2014 CMAQ simulation closely reflect the corresponding 8-hour observed ozone concentrations in space and time in each subregion of the 12-km modeling domain. As indicated by the statistics in Table 4-4, bias and error for 8-hour daily maximum ozone are relatively low in each subregion, not only in the summer when concentrations are highest, but also during other times of the year. Generally, 8-hour ozone at the AQS sites in the summer and fall is over predicted with the greatest over prediction in the South and Southeast (NMB ranging between 12 to 34 percent). Likewise, 8-hour ozone at the CASTNet sites in the summer is typically over predicted except in the West where the bias shows a slight under prediction (NMB of -0.3%). 8-hour ozone is under predicted at AQS and CASTNet sites in the Northeast and Upper Midwest in the winter and spring (with NMBs less than approximately 10 percent in each subregion).

Model bias at individual sites during the ozone season is similar to that seen on a subregional basis for the summer. Figure 4-2 shows the mean bias for 8-hour daily maximum ozone greater than 60 ppb is generally ±10 ppb across the AQS and CASTNet sites. Likewise, the information in Figure 4-4 indicates that the bias for days with observed 8-hour daily maximum ozone greater than 60 ppb is within ± 20 percent at the vast majority of monitoring sites across the U.S. domain. Model error, as seen from Figures 4-4 and 4-6, is generally 2 to 10 ppb and 20 percent or less at most of the sites across the U.S. modeling domain. Somewhat greater error is evident at sites in several areas most notably in the West, Northern Rockies, Northeast, Southeast, along portions of the Gulf Coast, and Great Lakes coastline.

**Table 4-4. Summary of CMAQ 2014 8-Hour Daily Maximum Ozone Model Performance Statistics by NOAA climate region, by Season and Monitoring Network.**

| Climate region | Monitor Network | Season | No. of Obs | MB (ppb) | ME (ppb) | NMB (%) | NME (%) |
|---|---|---|---|---|---|---|---|
| Northeast | AQS | Winter | 12,047 | -0.1 | 5.7 | -0.2 | 18.2 |

| Climate region | Monitor Network | Season | No. of Obs | MB (ppb) | ME (ppb) | NMB (%) | NME (%) |
|---|---|---|---|---|---|---|---|
| | | Spring | 16,172 | -0.3 | 5.3 | -0.7 | 12.0 |
| | | Summer | 17,263 | 6.6 | 7.9 | 15.2 | 18.2 |
| | | Fall | 14,720 | 8.7 | 9.3 | 26.4 | 28.1 |
| | | | | | | | |
| | CASTNet | Winter | 1,280 | -0.8 | 5.2 | -2.3 | 15.5 |
| | | Spring | 1,296 | -1.3 | 5.0 | -2.9 | 11.0 |
| | | Summer | 1,299 | 4.6 | 7.2 | 10.8 | 17.1 |
| | | Fall | 1,225 | 8.4 | 8.9 | 25.1 | 26.5 |
| | | | | | | | |
| Ohio Valley | AQS | Winter | 4,065 | 1.3 | 5.9 | 4.2 | 19.9 |
| | | Spring | 15,708 | 2.8 | 5.7 | 6.0 | 12.3 |
| | | Summer | 19,913 | 8.4 | 9.8 | 18.9 | 22.0 |
| | | Fall | 13,392 | 9.8 | 10.3 | 27.6 | 29.2 |
| | | | | | | | |
| | CASTNet | Winter | 1,583 | 1.2 | 6.2 | 3.5 | 18.8 |
| | | Spring | 1,634 | 0.2 | 5.4 | 0.3 | 11.0 |
| | | Summer | 1,627 | 2.2 | 13.6 | 4.5 | 27.5 |
| | | Fall | 1,609 | 7.8 | 9.0 | 21.5 | 24.9 |
| | | | | | | | |
| Upper Midwest | AQS | Winter | 1,495 | -1.8 | 6.6 | -5.8 | 21.5 |
| | | Spring | 6,916 | -0.1 | 5.4 | -0.2 | 11.8 |
| | | Summer | 9,538 | 4.4 | 7.2 | 10.7 | 17.4 |
| | | Fall | 5,941 | 8.1 | 8.9 | 24.3 | 26.6 |
| | | | | | | | |
| | CASTNet | Winter | 445 | -3.7 | 7.4 | -10.9 | 21.7 |
| | | Spring | 457 | -3.1 | 6.0 | -6.7 | 12.8 |
| | | Summer | 458 | 2.0 | 5.8 | 5.0 | 14.5 |
| | | Fall | 444 | 6.6 | 7.6 | 20.2 | 23.3 |
| | | | | | | | |
| Southeast | AQS | Winter | 6,723 | 5.9 | 7.2 | 17.6 | 21.3 |
| | | Spring | 14,962 | 4.2 | 6.6 | 9.0 | 14.1 |
| | | Summer | 16,998 | 13.5 | 14.0 | 33.5 | 34.7 |
| | | Fall | 13,787 | 12.6 | 12.8 | 34.8 | 35.4 |
| | | | | | | | |
| | CASTNet | Winter | 946 | 2.6 | 5.7 | 7.1 | 15.6 |
| | | Spring | 998 | -0.2 | 6.3 | -0.5 | 12.5 |
| | | Summer | 998 | 9.9 | 10.6 | 23.9 | 25.7 |
| | | Fall | 975 | 9.3 | 10.1 | 25.0 | 27.1 |
| | | | | | | | |
| South | AQS | Winter | 12,064 | 4.5 | 6.4 | 14.6 | 20.6 |
| | | Spring | 13,851 | 5.1 | 7.4 | 11.5 | 16.6 |
| | | Summer | 13,756 | 17.9 | 18.5 | 45.8 | 47.2 |
| | | Fall | 13,265 | 10.7 | 11.4 | 28.6 | 30.3 |

| Climate region | Monitor Network | Season | No. of Obs | MB (ppb) | ME (ppb) | NMB (%) | NME (%) |
|---|---|---|---|---|---|---|---|
| | | | | | | | |
| | CASTNet | Winter | 518 | 3.6 | 5.8 | 10.4 | 16.8 |
| | | Spring | 551 | 3.1 | 6.3 | 6.5 | 13.4 |
| | | Summer | 537 | 11.2 | 15.8 | 26.4 | 37.2 |
| | | Fall | 530 | 10.4 | 10.8 | 28.3 | 29.2 |
| | | | | | | | |
| Southwest | AQS | Winter | 9,341 | 4.8 | 7.2 | 13.2 | 19.8 |
| | | Spring | 11,234 | 3.0 | 5.5 | 5.7 | 10.4 |
| | | Summer | 11,517 | 9.3 | 11.3 | 17.8 | 21.6 |
| | | Fall | 10,311 | 12.4 | 12.6 | 29.3 | 29.9 |
| | | | | | | | |
| | CASTNet | Winter | 774 | 1.1 | 6.1 | 2.5 | 13.8 |
| | | Spring | 817 | 0.2 | 5.8 | 0.4 | 10.3 |
| | | Summer | 817 | 7.1 | 10.3 | 13.1 | 18.9 |
| | | Fall | 801 | 10.3 | 11.3 | 22.4 | 24.6 |
| | | | | | | | |
| Northern Rockies | AQS | Winter | 4,553 | -0.4 | 6.0 | -1.2 | 16.5 |
| | | Spring | 4,898 | 1.8 | 5.0 | 3.8 | 10.8 |
| | | Summer | 4,872 | 5.5 | 7.3 | 12.1 | 16.2 |
| | | Fall | 4,799 | 9.1 | 9.7 | 24.2 | 25.8 |
| | | | | | | | |
| | CASTNet | Winter | 607 | -1.2 | 5.2 | -3.0 | 13.3 |
| | | Spring | 637 | -0.6 | 4.8 | -1.2 | 9.6 |
| | | Summer | 628 | 3.2 | 7.1 | 6.8 | 14.9 |
| | | Fall | 611 | 8.4 | 9.3 | 20.8 | 23.0 |
| | | | | | | | |
| Northwest | AQS | Winter | 596 | 5.4 | 7.4 | 18.5 | 25.5 |
| | | Spring | 1,194 | 0.3 | 4.7 | 0.7 | 11.6 |
| | | Summer | 2,404 | 5.5 | 8.3 | 14.5 | 21.6 |
| | | Fall | 1,258 | 8.7 | 9.8 | 25.4 | 28.6 |
| | | | | | | | |
| | CASTNet | Winter | -- | -- | -- | -- | -- |
| | | Spring | -- | -- | -- | -- | -- |
| | | Summer | -- | -- | -- | -- | -- |
| | | Fall | -- | -- | -- | -- | -- |
| | | | | | | | |
| West | AQS | Winter | 14,984 | 6.3 | 8.3 | 19.0 | 24.8 |
| | | Spring | 16,829 | 0.8 | 5.4 | 1.6 | 10.8 |
| | | Summer | 17,881 | 6.0 | 10.0 | 11.9 | 20.0 |
| | | Fall | 16,611 | 8.4 | 10.0 | 18.7 | 22.3 |
| | | | | | | | |
| | CASTNet | Winter | 530 | 4.5 | 7.0 | 10.8 | 16.8 |
| | | Spring | 552 | -3.0 | 6.2 | -5.4 | 11.1 |

| Climate region | Monitor Network | Season | No. of Obs | MB (ppb) | ME (ppb) | NMB (%) | NME (%) |
|---|---|---|---|---|---|---|---|
| | | Summer | 542 | -0.2 | 10.6 | -0.3 | 17.8 |
| | | Fall | 538 | 6.4 | 11.0 | 12.7 | 21.8 |

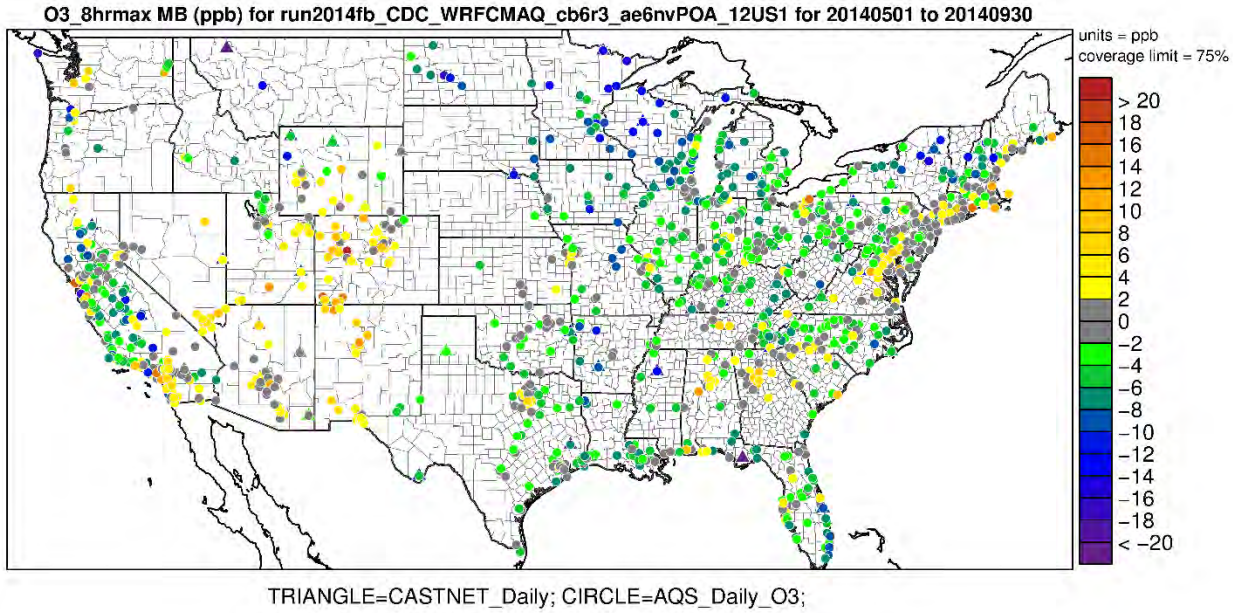



**Figure 4-3. Mean Bias (ppb) of 8-hour daily maximum ozone greater than 60 ppb over the period May-September 2014 at AQS and CASTNet monitoring sites in the continental U.S. modeling domain.**

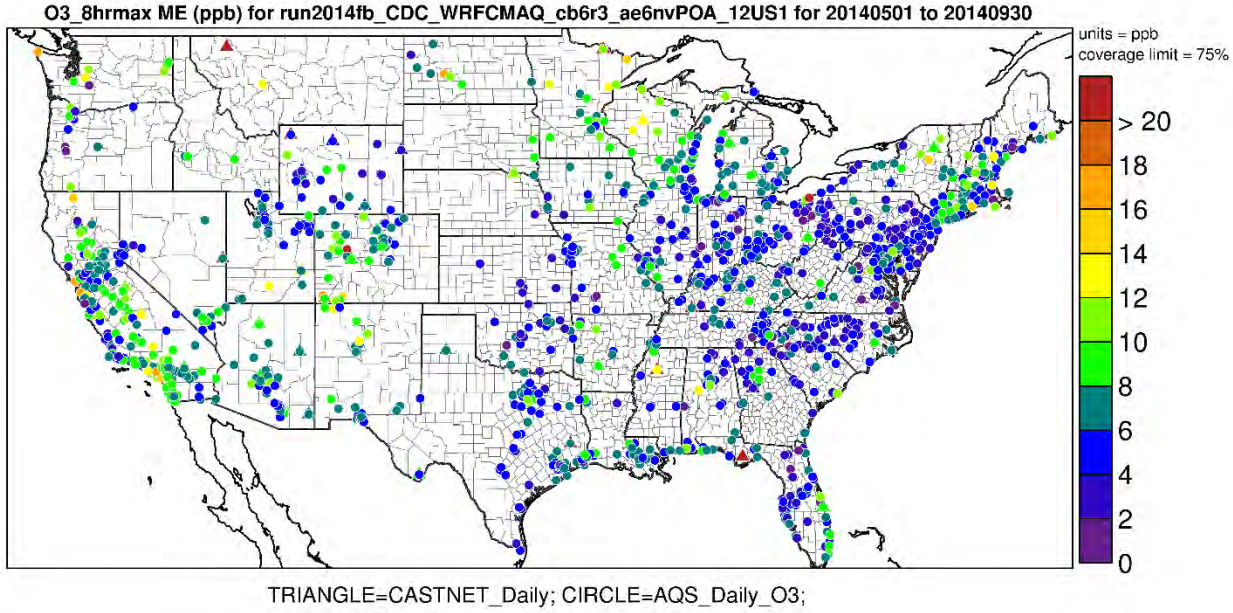



**Figure 4-4. Mean Error (ppb) of 8-hour daily maximum ozone greater than 60 ppb over the period May-September 2014 at AQS and CASTNet monitoring sites in the continental U.S. modeling**

**domain.**

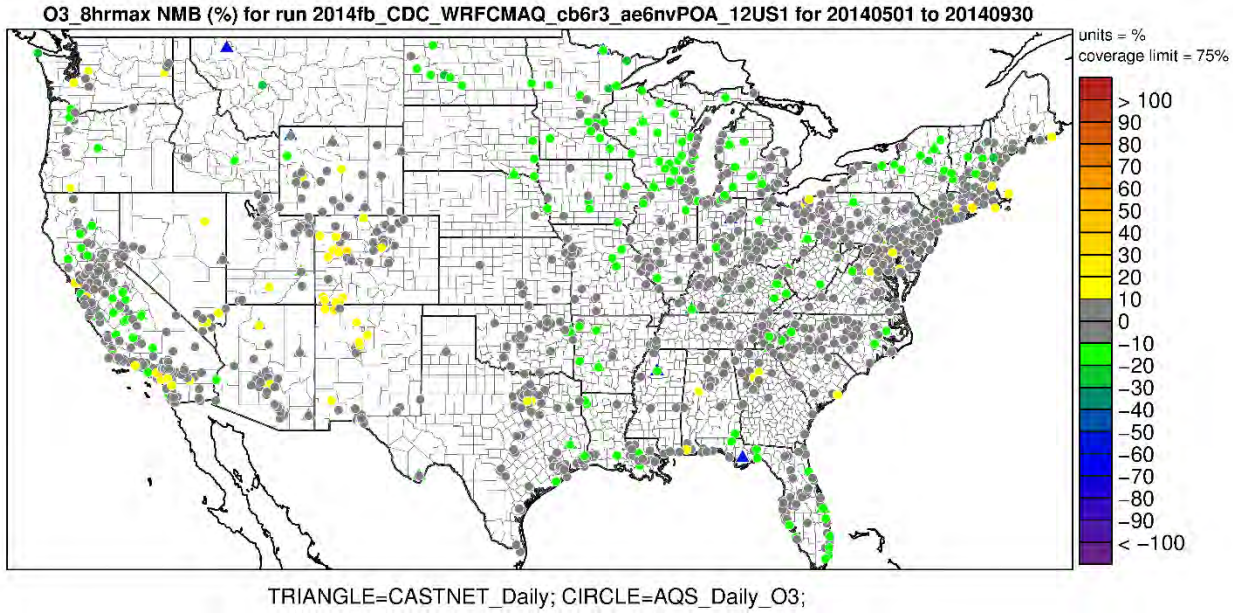



**Figure 4-5. Normalized Mean Bias (%) of 8-hour daily maximum ozone greater than 60 ppb over the period May-September 2014 at AQS and CASTNet monitoring sites in the continental U.S. modeling domain.**

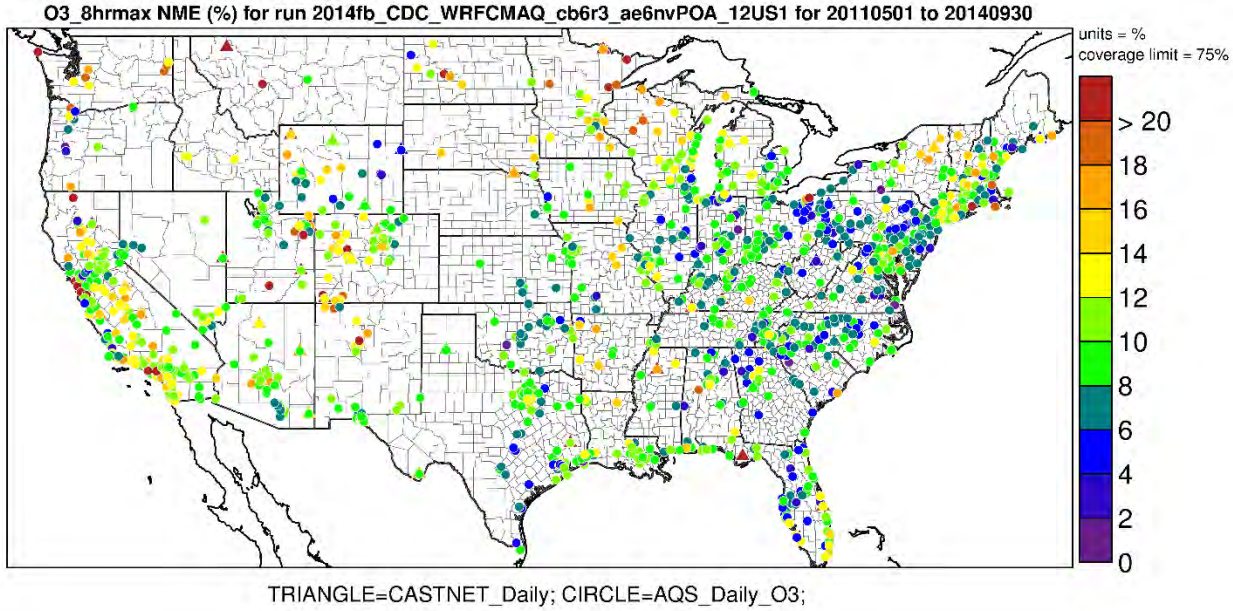



**Figure 4-6. Normalized Mean Error (%) of 8-hour daily maximum ozone greater than 60 ppb over the period May-September 2014 at AQS and CASTNet monitoring sites in the continental U.S. modeling domain.**

*Evaluation for Annual $PM_{2.5}$ components:* The PM evaluation focuses on $PM_{2.5}$ components including sulfate ($SO_4$), nitrate ($NO_3$), total nitrate ($TNO_3 = NO_3 + HNO_3$), ammonium ($NH_4$), elemental carbon

(EC), and organic carbon (OC). The bias and error performance statistics were calculated on an annual basis for each of the nine NOAA climate subregions defined above (provided in Table 4-5). $PM_{2.5}$ measurements for 2014 were obtained from the following networks for model evaluation: Chemical Speciation Network (CSN, 24-hour average), Interagency Monitoring of Protected Visual Environments (IMPROVE, 24-hour average, and Clean Air Status and Trends Network (CASTNet, weekly average). For $PM_{2.5}$ species that are measured by more than one network, we calculated separate sets of statistics for each network by subregion. In addition to the tabular summaries of bias and error statistics, annual spatial maps which show the mean bias, mean error, normalized mean bias and normalized mean error by site for each $PM_{2.5}$ species are provided in Figures 4-7 through 4-30.

As indicated by the statistics in Table 4-5, annual average sulfate is consistently under predicted at CSN, IMPROVE, and CASTNet monitoring sites across the 12-km modeling domain (with MB values ranging from 0.0 to -0.6 $\mu gm^{-3}$ and NMB values ranging from near negligible to -32 percent) except at CSN sites in the Southeast, Northern Rockies and Northwest as well as IMPROVE sites in the Northwest (over predicted NMB ranges between 1 to 38 percent). Sulfate performance shows moderate error, ranging from 26 to 66 percent. Figures 4-7 through 4-10, suggest spatial patterns vary by region. The model bias for most of the Northeast, Southeast, Central and Southwest states are within ±30 percent. The model bias appears to be slightly greater in the Northwest with over predictions up to 80 percent at individual monitors. Model error also shows a spatial trend by region, where much of the Eastern states are 20 to 40 percent, the Western and Central U.S. states are 30 to 80 percent.

Annual average nitrate is under predicted at the urban CSN monitoring sites in the Ohio Valley, Upper Midwest, South, Southwest, Northern Rockies, and West (NMB in the range of -17.0 to -49 percent), except in the Northeast, Northwest, and Southeast where nitrate is over predicted (NMB in the range of 7 percent and 49 percent). At IMPROVE rural sites, annual average nitrate is under predicted at all subregions, except in the Southeast, Northeast, and Northwest where nitrate is over predicted by 23 to 34 percent, respectively. Model performance of total nitrate at sub-urban CASTNet monitoring sites shows an over prediction in the Northeast, Ohio Valley, Upper Midwest, South, Southwest, and Southeast (NMB in the range of 1 to 40 percent), except in the Northern Rockies and Western U.S. (NMB in the range of -12 to -27 percent). Model error for nitrate and total nitrate is somewhat greater for each of the nine NOAA climate subregions as compared to sulfate. Model bias at individual sites indicates mainly over prediction of greater than 20 percent at most monitoring sites in the Eastern half of the U.S. as indicated in Figure 4-13. The exception to this is in the Southern Florida, Ohio Valley, Southwest, and Western U.S. of the modeling domain where there appears to be a greater number of sites with under prediction of nitrate of 10 to 80 percent. Model error for annual nitrate, as shown in Figures 4-12 and 4-15, is least at sites in portions of the Southeast and extending upward to the Northeast corridor. Nitrate concentrations are typically higher in these areas than in other portions of the modeling domain.

Annual average ammonium model performance as indicated in Table 4-5 has a tendency for the model to under predict across the CASTNet sites (ranging from -19 to -49 percent. Likewise, ammonium performance across the urban CSN sites shows an under prediction in most of the climate subregions (ranging from -8 to -45 percent), except in the Northeast, Northwest and Southeast (over prediction of NMB 5 and 38 percent, respectively). The spatial variation of ammonium across the majority of individual monitoring sites in the Eastern U.S. shows bias within ±50 percent (Figures 4-19 and 4-21). A larger bias is seen in the Southeast and in the Northern Rockies, (over prediction bias on average 80 percent). The urban monitoring sites exhibit larger errors than at rural sites for ammonium.

Annual average elemental carbon is over predicted in all of the nine subregions at urban and rural sites.

There is not a large variation in error statistics from subregion to subregion or at urban versus rural sites.

Annual average organic carbon is over predicted across most subregions in rural IMPROVE areas (NMB ranging from 3 to 47 percent), except in the Southwest, Northern Rockies, and Western U.S. where the bias ranges between -8 to -31 percent. The model over predicted annual average organic carbon in all subregions at urban CSN sites except in the Northern Rockies and Western U.S. (NMB ranges from -8 to -19 percent). Similar to elemental carbon, error model performance does not show a large variation from subregion to subregion or at urban versus rural sites.

**Table 4-5. Summary of CMAQ 2014 Annual PM Species Model Performance Statistics by NOAA Climate region, by Monitoring Network.**

| Pollutant | Monitor Network | Subregion | No. of Obs | MB ($\mu gm^{-3}$) | ME ($\mu gm^{-3}$) | NMB (%) | NME (%) |
|---|---|---|---|---|---|---|---|
| Sulfate | CSN | Northeast | 906 | -0.3 | 0.6 | -17.0 | 35.2 |
| | | Ohio Valley | 3,037 | -0.4 | 0.7 | -17.6 | 35.0 |
| | | Upper Midwest | 1,604 | -0.1 | 0.5 | -9.4 | 34.1 |
| | | Southeast | 2,066 | 0.0 | 0.6 | 1.0 | 34.5 |
| | | South | 1,456 | -0.3 | 0.6 | -19.0 | 34.6 |
| | | Southwest | 783 | -0.1 | 0.3 | -9.7 | 43.1 |
| | | Northern Rockies | 570 | 0.0 | 0.4 | 2.8 | 51.9 |
| | | Northwest | 620 | 0.1 | 0.4 | 15.2 | 55.6 |
| | | West | 956 | -0.2 | 0.3 | -15.3 | 39.6 |
| | | | | | | | |
| | IMPROVE | Northeast | 1,714 | -0.1 | 0.3 | -11.3 | 33.0 |
| | | Ohio Valley | 797 | -0.3 | 0.5 | -14.0 | 30.1 |
| | | Upper Midwest | 938 | -0.1 | 0.4 | -7.6 | 36.1 |
| | | Southeast | 1,147 | -0.1 | 0.5 | -6.6 | 30.1 |
| | | South | 1,164 | -0.3 | 0.5 | -19.1 | 36.1 |
| | | Southwest | 3,803 | -0.1 | 0.2 | -17.0 | 42.5 |
| | | Northern Rockies | 2,121 | 0.0 | 0.2 | 0.8 | 45.8 |
| | | Northwest | 1,822 | 0.1 | 0.2 | 38.1 | 65.8 |
| | | West | 2,400 | 0.0 | 0.3 | -4.5 | 50.2 |
| | | | | | | | |
| | CASTNet | Northeast | 906 | -0.3 | 0.4 | -23.6 | 27.2 |
| | | Ohio Valley | 893 | -0.6 | 0.6 | -25.1 | 27.2 |
| | | Upper Midwest | 257 | -0.3 | 0.4 | -21.9 | 26.0 |
| | | Southeast | 586 | -0.5 | 0.5 | -25.0 | 27.9 |
| | | South | 377 | -0.6 | 0.6 | -30.7 | 32.2 |
| | | Southwest | 422 | -0.1 | 0.2 | -24.3 | 39.1 |
| | | Northern Rockies | 566 | -0.1 | 0.2 | -20.1 | 36.3 |
| | | Northwest | - | - | - | - | - |
| | | West | 296 | -0.2 | 0.3 | -31.8 | 45.7 |
| Nitrate | CSN | Northeast | 3,237 | 0.1 | 0.7 | 7.2 | 56.5 |
| | | Ohio Valley | 2,841 | -0.3 | 0.9 | -18.3 | 55.5 |
| | | Upper Midwest | 1,604 | -0.3 | 0.8 | -16.9 | 46.9 |
| | | Southeast | 2,308 | 0.3 | 0.5 | 49.9 | 98.1 |

| Pollutant | Monitor Network | Subregion | No. of Obs | MB ($\mu gm^{-3}$) | ME ($\mu gm^{-3}$) | NMB (%) | NME (%) |
|---|---|---|---|---|---|---|---|
| | | South | 1,238 | -0.2 | 0.6 | -20.1 | 70.4 |
| | | Southwest | 783 | -0.3 | 0.9 | -29.1 | 80.5 |
| | | Northern Rockies | 570 | -0.4 | 0.6 | -34.3 | 59.1 |
| | | Northwest | 523 | 0.2 | 0.8 | 27.4 | 98.5 |
| | | West | 956 | -1.2 | 1.5 | -49.3 | 65.8 |
| | | | | | | | |
| | IMPROVE | Northeast | 1,709 | 0.1 | 0.3 | 33.8 | 83.7 |
| | | Ohio Valley | 797 | -0.2 | 0.6 | -17.7 | 69.1 |
| | | Upper Midwest | 938 | -0.2 | 0.6 | -17.4 | 59.2 |
| | | Southeast | 1,147 | 0.1 | 0.4 | 27.1 | 96.8 |
| | | South | 1,164 | -0.2 | 0.5 | -25.8 | 75.6 |
| | | Southwest | 3,801 | -0.1 | 0.2 | -28.5 | 91.1 |
| | | Northern Rockies | 2,120 | -0.1 | 0.2 | -36.2 | 79.3 |
| | | Northwest | 1,807 | 0.0 | 0.2 | 23.3 | >100.0 |
| | | West | 2,390 | -0.3 | 0.5 | -49.9 | 79.9 |
| | | | | | | | |
| Total Nitrate ($NO_3$+$HNO_3$) | CASTNet | Northeast | 906 | 0.3 | 0.5 | 23.6 | 37.9 |
| | | Ohio Valley | 893 | 0.3 | 0.9 | 16.1 | 43.0 |
| | | Upper Midwest | 257 | 0.0 | 0.6 | 1.1 | 34.9 |
| | | Southeast | 586 | 0.5 | 0.8 | 38.9 | 64.6 |
| | | South | 377 | 0.3 | 0.8 | 19.7 | 51.9 |
| | | Southwest | 422 | 0.1 | 0.3 | 11.0 | 41.8 |
| | | Northern Rockies | 566 | -0.1 | 0.3 | -11.8 | 37.5 |
| | | Northwest | - | - | - | - | - |
| | | West | 296 | -0.4 | 0.7 | -26.5 | 47.1 |
| | | | | | | | |
| Ammonium | CSN | Northeast | 3,237 | 0.0 | 0.3 | 4.9 | 48.3 |
| | | Ohio Valley | 2,744 | -0.2 | 0.4 | -17.0 | 45.0 |
| | | Upper Midwest | 1,475 | -0.1 | 0.4 | -8.4 | 42.8 |
| | | Southeast | 1,803 | 0.1 | 0.3 | 17.0 | 56.8 |
| | | South | 1,230 | -0.1 | 0.3 | -20.8 | 49.2 |
| | | Southwest | 765 | -0.2 | 0.3 | -45.2 | 67.7 |
| | | Northern Rockies | 570 | -0.1 | 0.3 | -11.0 | 56.4 |
| | | Northwest | 610 | 0.1 | 0.3 | 37.5 | >100.0 |
| | | West | 945 | -0.3 | 0.5 | -43.4 | 64.4 |
| | | | | | | | |
| | CASTNet | Northeast | 906 | -0.1 | 0.2 | -19.0 | 28.8 |
| | | Ohio Valley | 893 | -0.3 | 0.3 | -27.6 | 35.0 |
| | | Upper Midwest | 257 | -0.2 | 0.3 | -27.5 | 34.6 |
| | | Southeast | 586 | -0.1 | 0.2 | -15.9 | 28.0 |
| | | South | 377 | -0.2 | 0.2 | -26.8 | 36.6 |
| | | Southwest | 422 | -0.1 | 0.1 | -43.1 | 53.1 |
| | | Northern Rockies | 566 | -0.1 | 0.1 | -42.8 | 51.0 |

| Pollutant | Monitor Network | Subregion | No. of Obs | MB ($\mu gm^{-3}$) | ME ($\mu gm^{-3}$) | NMB (%) | NME (%) |
|---|---|---|---|---|---|---|---|
| | | Northwest | - | - | - | - | - |
| | | West | 296 | -0.1 | 0.2 | -49.3 | 59.9 |
| | | | | | | | |
| Elemental Carbon | CSN | Northeast | 3,186 | 0.3 | 0.5 | 50.4 | 76.4 |
| | | Ohio Valley | 2,723 | 0.2 | 0.3 | 35.2 | 62.9 |
| | | Upper Midwest | 1,434 | 0.2 | 0.3 | 54.4 | 70.8 |
| | | Southeast | 1,766 | 0.3 | 0.4 | 49.9 | 73.6 |
| | | South | 1,218 | 0.2 | 0.3 | 35.4 | 55.4 |
| | | Southwest | 769 | 0.3 | 0.4 | 51.7 | 71.3 |
| | | Northern Rockies | 546 | 0.1 | 0.3 | 24.2 | 86.8 |
| | | Northwest | 583 | 0.7 | 0.9 | >100.0 | >100.0 |
| | | West | 870 | 0.0 | 0.4 | 5.0 | 50.2 |
| | | | | | | | |
| | IMPROVE | Northeast | 1,730 | 0.1 | 0.1 | 43.9 | 65.2 |
| | | Ohio Valley | 806 | 0.1 | 0.1 | 25.3 | 58.2 |
| | | Upper Midwest | 945 | 0.1 | 0.1 | 26.0 | 57.1 |
| | | Southeast | 1,349 | 0.1 | 0.2 | 41.4 | 64.2 |
| | | South | 1,160 | 0.0 | 0.1 | 25.7 | 54.9 |
| | | Southwest | 3,793 | 0.0 | 0.1 | 34.2 | 72.2 |
| | | Northern Rockies | 2,270 | 0.0 | 0.1 | 10.0 | 63.7 |
| | | Northwest | 1,815 | 0.2 | 0.3 | >100.0 | >100.0 |
| | | West | 2,391 | 0.1 | 0.1 | 39.5 | 83.0 |
| | | | | | | | |
| Organic Carbon | CSN | Northeast | 3,146 | 2.3 | 2.5 | >100.0 | >100.0 |
| | | Ohio Valley | 2,692 | 0.5 | 0.9 | 32.9 | 56.6 |
| | | Upper Midwest | 1,426 | 0.9 | 1.2 | 59.7 | 84.8 |
| | | Southeast | 1,755 | 1.2 | 1.5 | 63.4 | 81.1 |
| | | South | 1,212 | 0.4 | 0.9 | 23.2 | 51.9 |
| | | Southwest | 768 | 0.9 | 1.2 | 67.4 | 89.3 |
| | | Northern Rockies | 510 | -0.2 | 0.9 | -18.5 | 72.2 |
| | | Northwest | 579 | 1.7 | 2.3 | 85.0 | >100.0 |
| | | West | 869 | -0.2 | 1.1 | -8.7 | 44.3 |
| | | | | | | | |
| | IMPROVE | Northeast | 1,724 | 0.3 | 0.6 | 34.4 | 68.6 |
| | | Ohio Valley | 806 | 0.3 | 0.7 | 28.2 | 59.6 |
| | | Upper Midwest | 940 | 0.2 | 0.6 | 20.5 | 68.9 |
| | | Southeast | 1,349 | 0.6 | 1.0 | 47.2 | 77.2 |
| | | South | 1,159 | 0.0 | 0.5 | 2.6 | 50.5 |
| | | Southwest | 3,780 | -0.1 | 0.3 | -10.5 | 56.4 |
| | | Northern Rockies | 2,252 | -0.2 | 0.4 | -31.1 | 57.7 |
| | | Northwest | 1,768 | 0.3 | 0.9 | 42.1 | >100.0 |
| | | West | 2,388 | -0.1 | 0.6 | -8.1 | 63.5 |

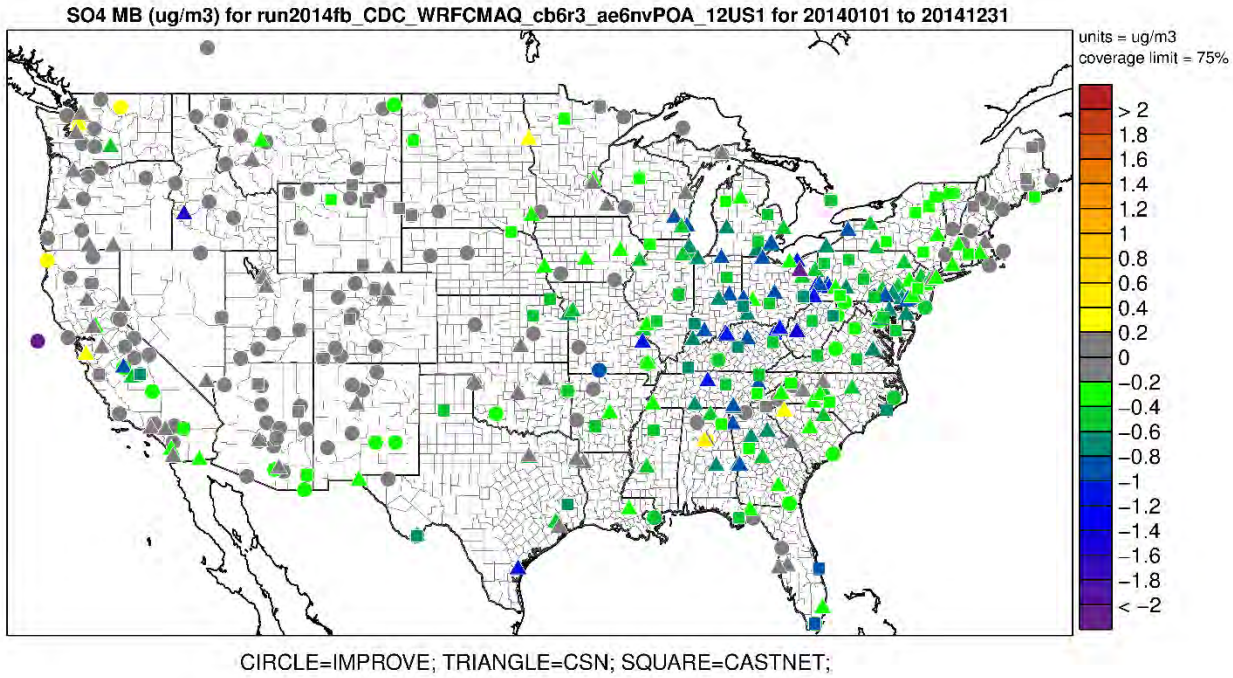



**Figure 4-7. Mean Bias (μgm$^{-3}$) of annual sulfate at monitoring sites in the continental U.S. modeling domain.**

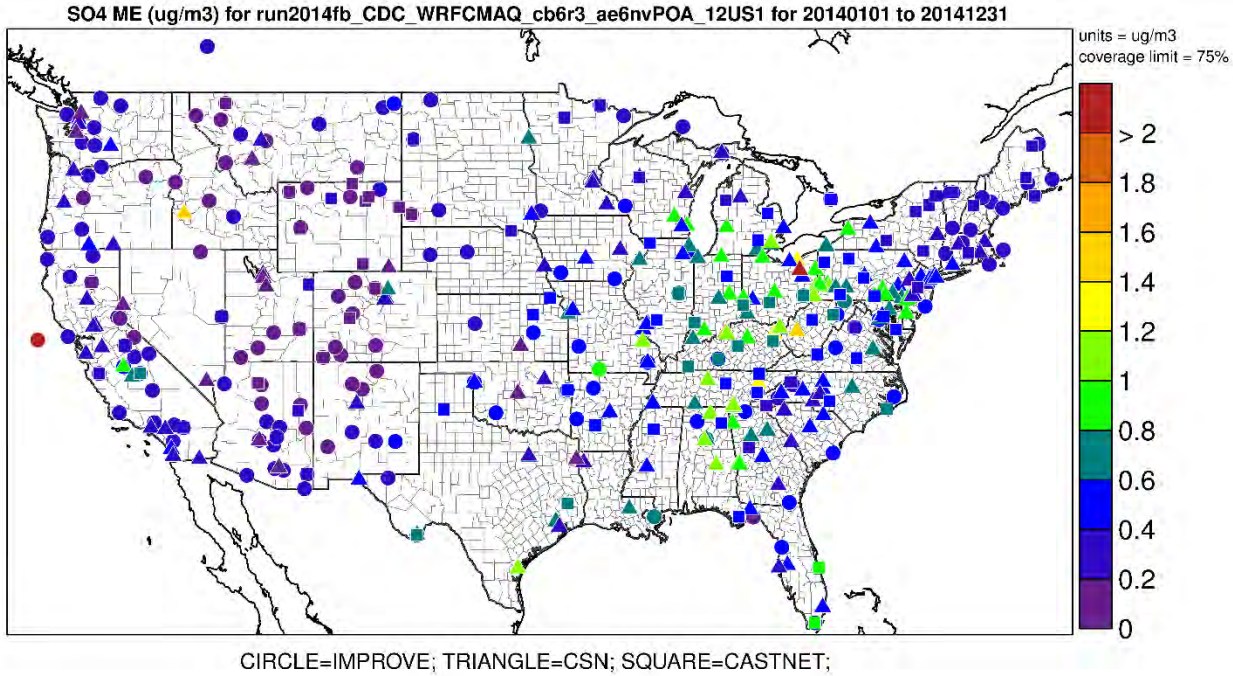



**Figure 4-8. Mean Error (μgm$^{-3}$) of annual sulfate at monitoring sites in the continental U.S. modeling domain.**

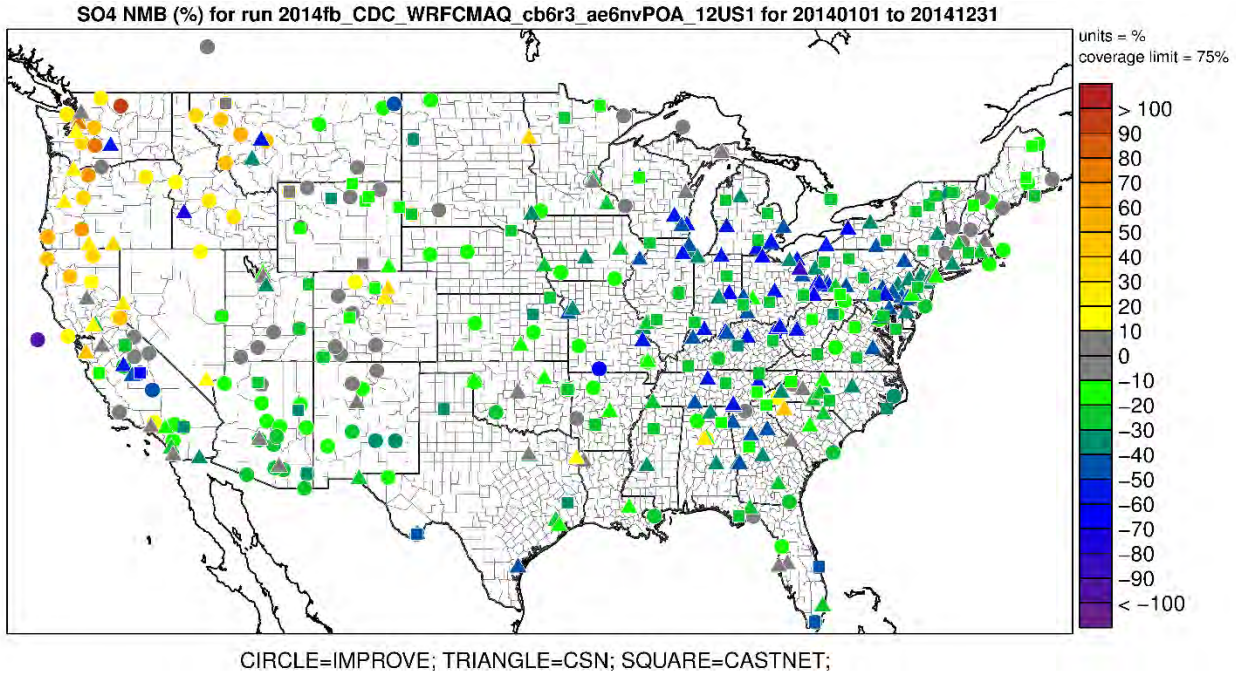



**Figure 4-9. Normalized Mean Bias (%) of annual sulfate at monitoring sites in the continental U.S. modeling domain.**

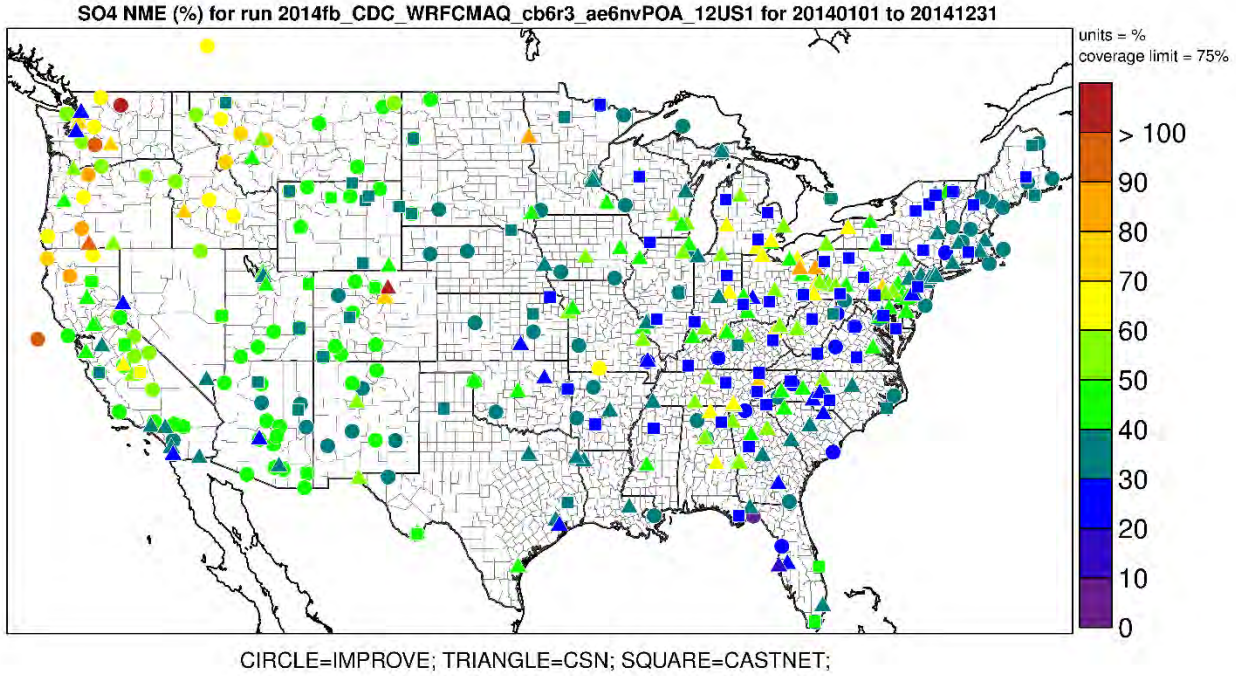



**Figure 4-10. Normalized Mean Error (%) of annual sulfate at monitoring sites in the continental U.S. modeling domain.**

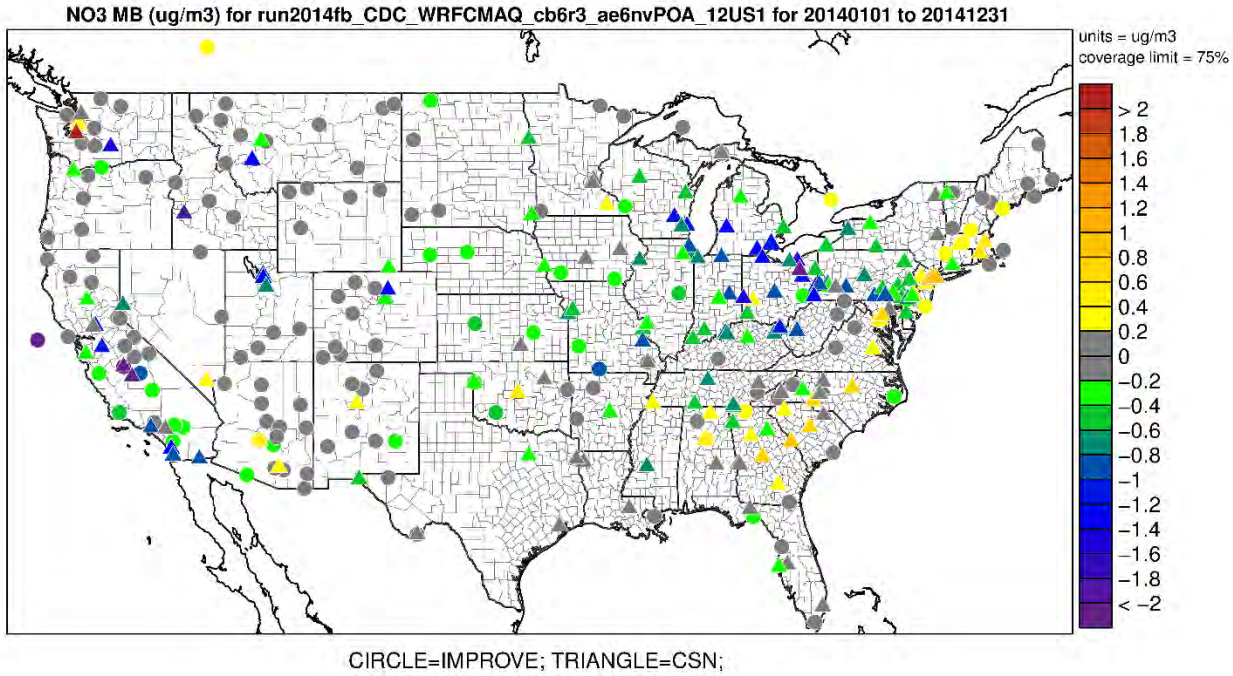



**Figure 4-11. Mean Bias ($\mu gm^{-3}$) of annual nitrate at monitoring sites in the continental U.S. modeling domain.**

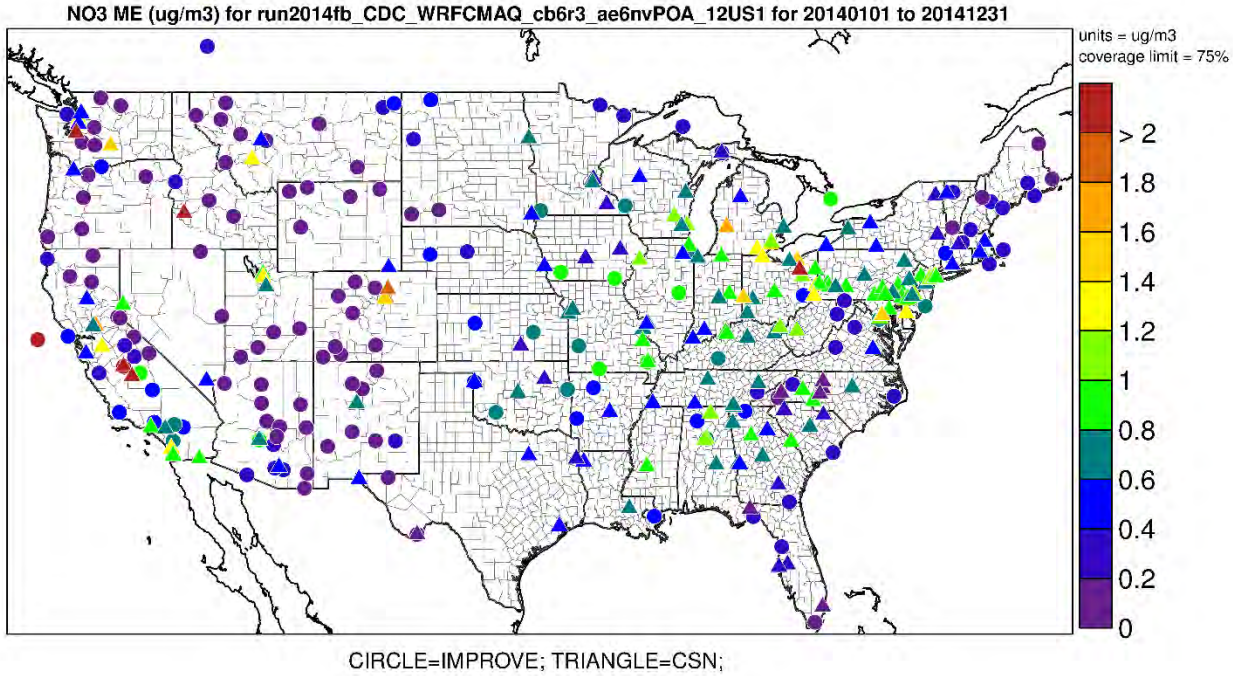



**Figure 4-12. Mean Error ($\mu gm^{-3}$) of annual nitrate at monitoring sites in the continental U.S. modeling domain.**

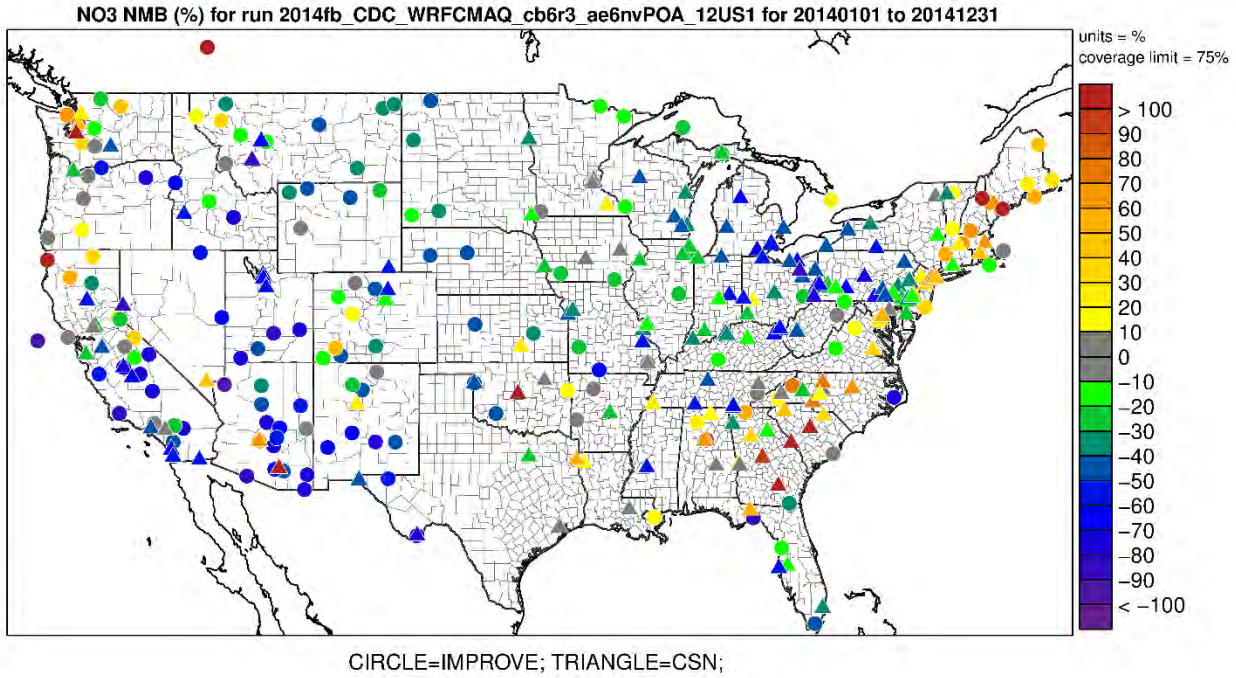



**Figure 4-13. Normalized Mean Bias (%) of annual nitrate at monitoring sites in the continental U.S. modeling domain.**

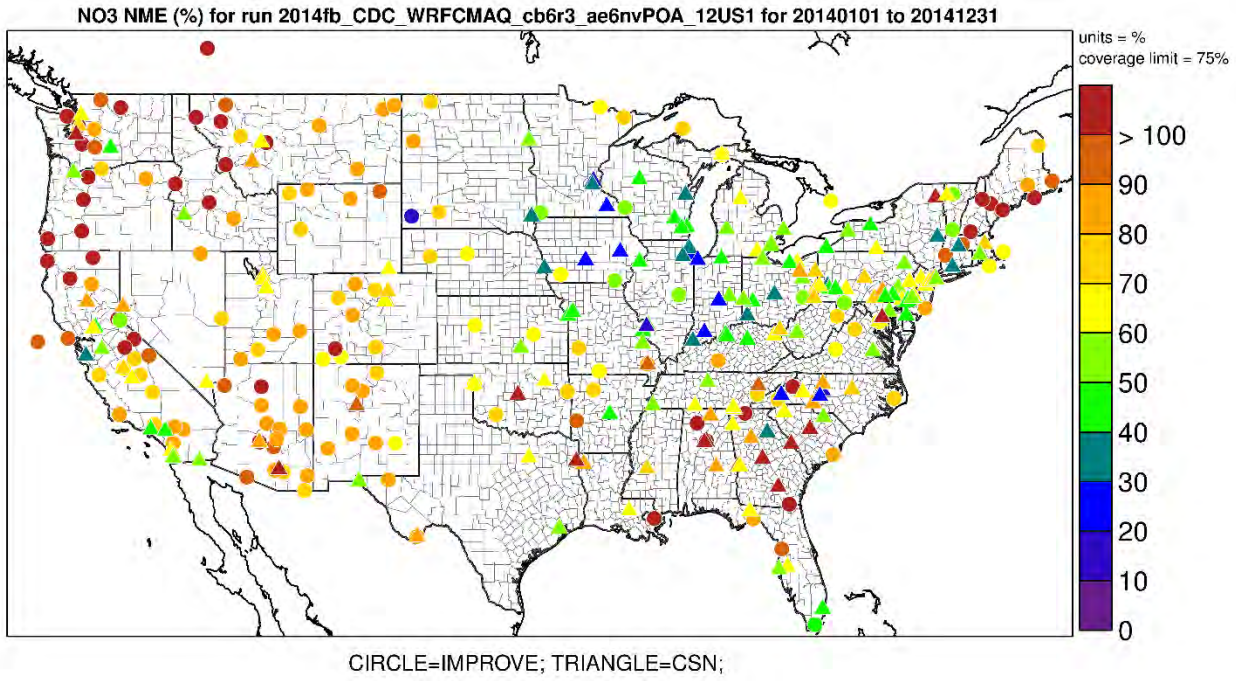



**Figure 4-14. Normalized Mean Error (%) of annual nitrate at monitoring sites in the continental U.S. modeling domain.**

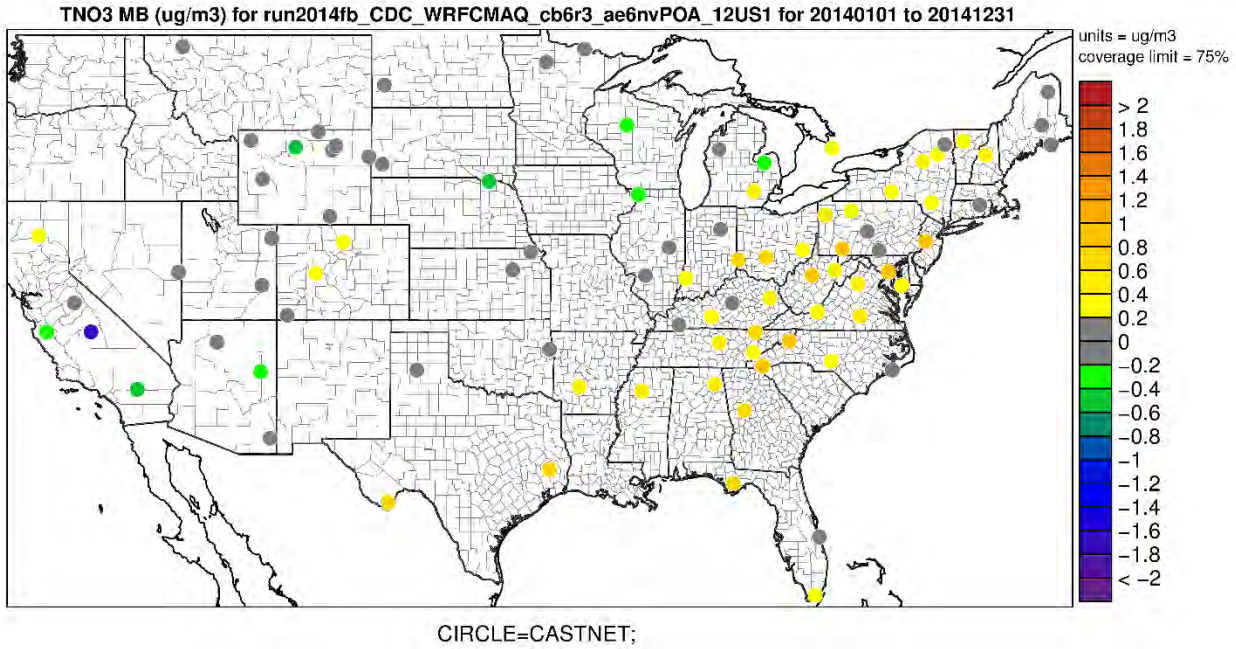



**Figure 4-15. Mean Bias (μgm$^{-3}$) of annual total nitrate at monitoring sites in the continental U.S. modeling domain.**

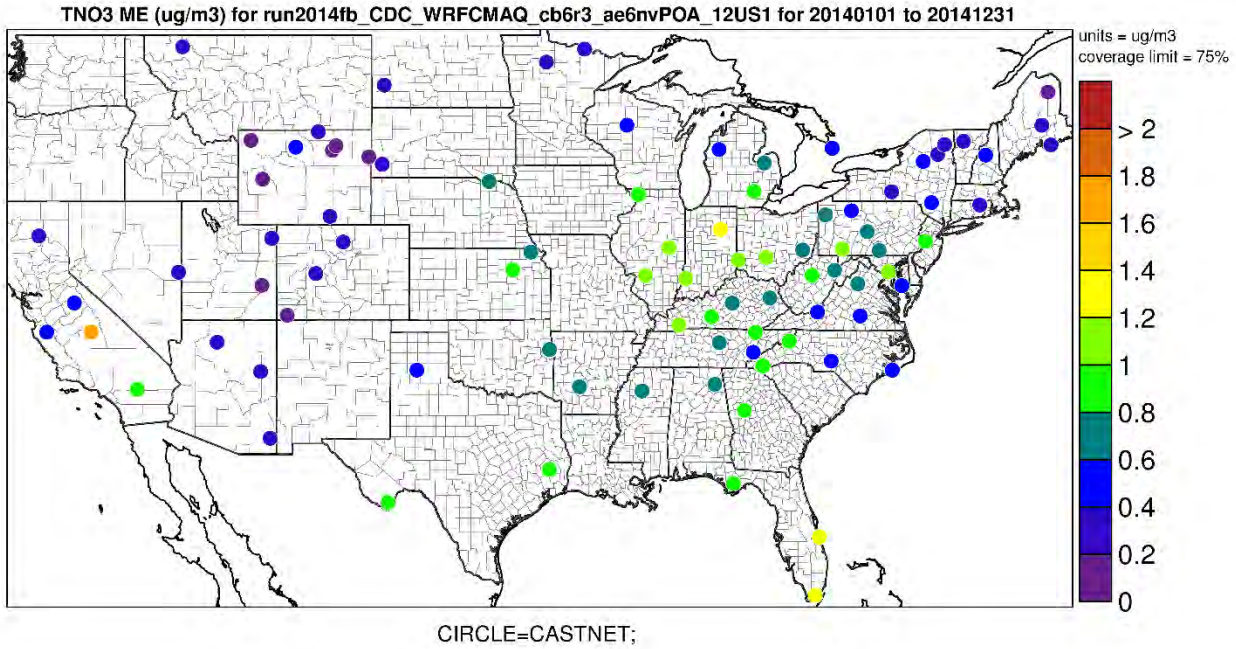



**Figure 4-16. Mean Error (μgm$^{-3}$) of annual total nitrate at monitoring sites in the continental U.S. modeling domain.**

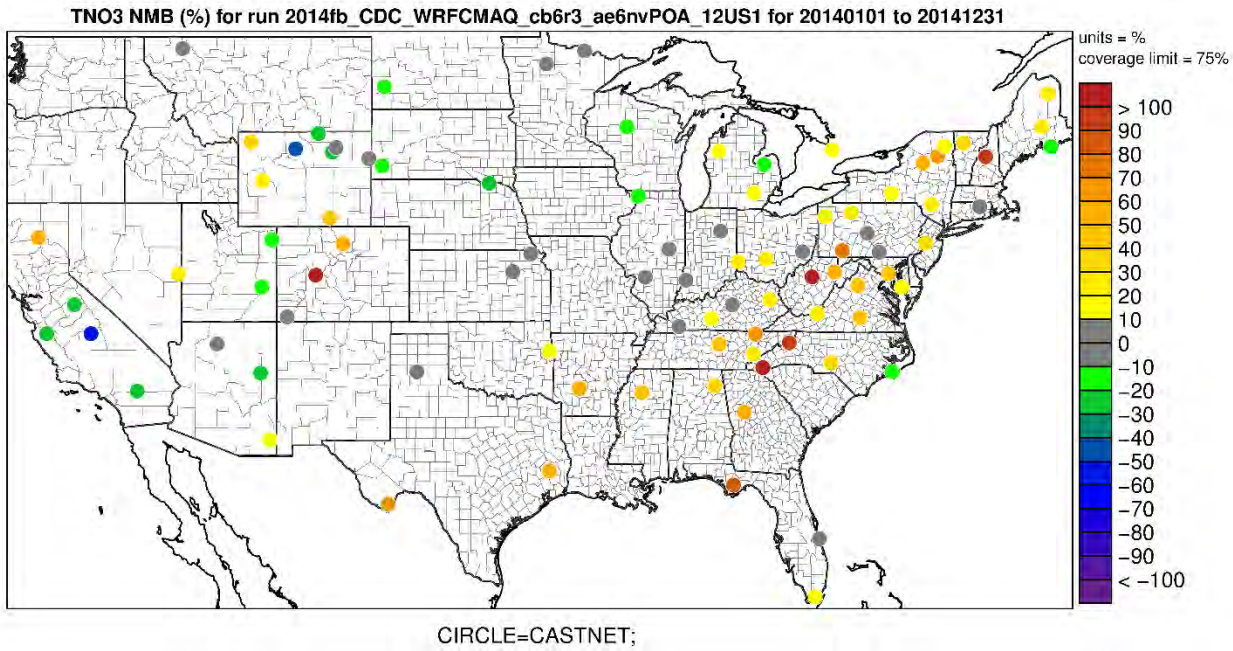



**Figure 4-17. Normalized Mean Bias (%) of annual total nitrate at monitoring sites in the continental U.S. modeling domain.**

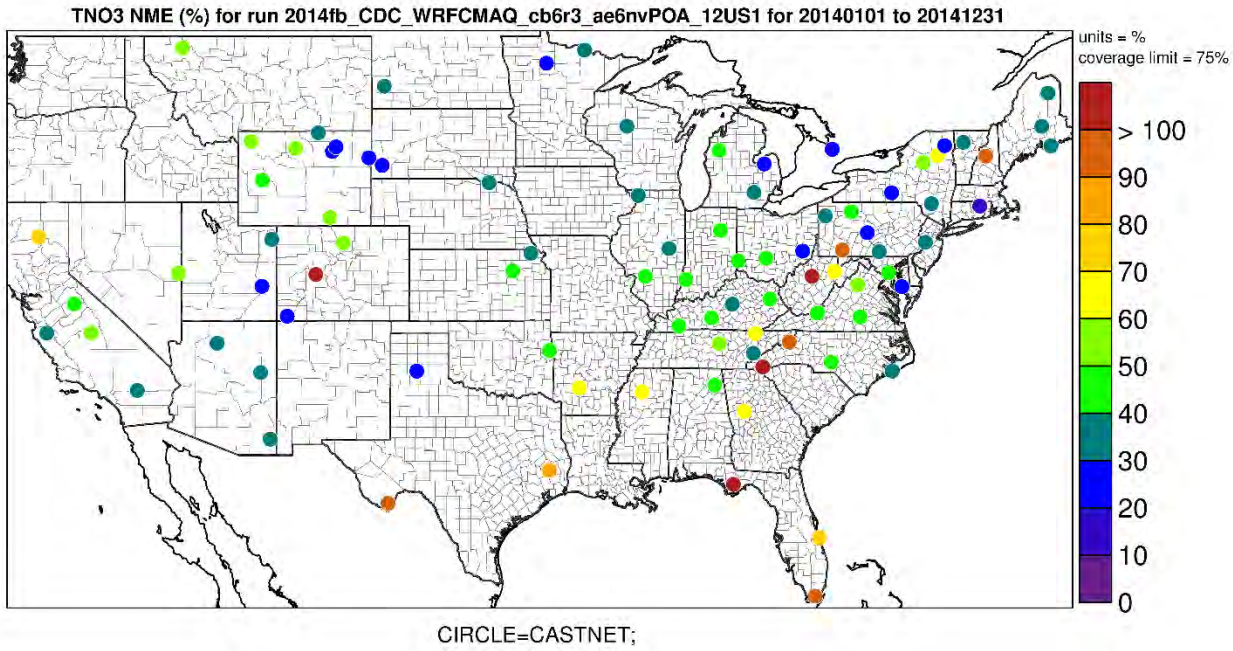



**Figure 4-18. Normalized Mean Error (%) of annual total nitrate at monitoring sites in the continental U.S. modeling domain.**

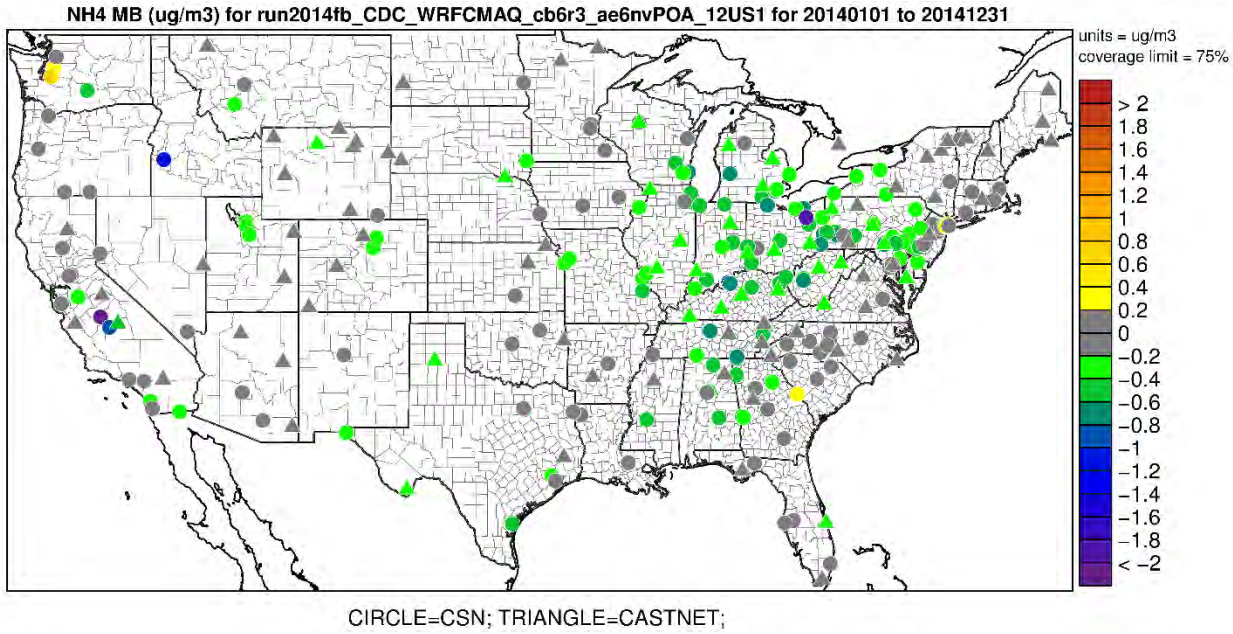



**Figure 4-19. Mean Bias (µgm$^{-3}$) of annual ammonium at monitoring sites in the continental U.S. modeling domain.**

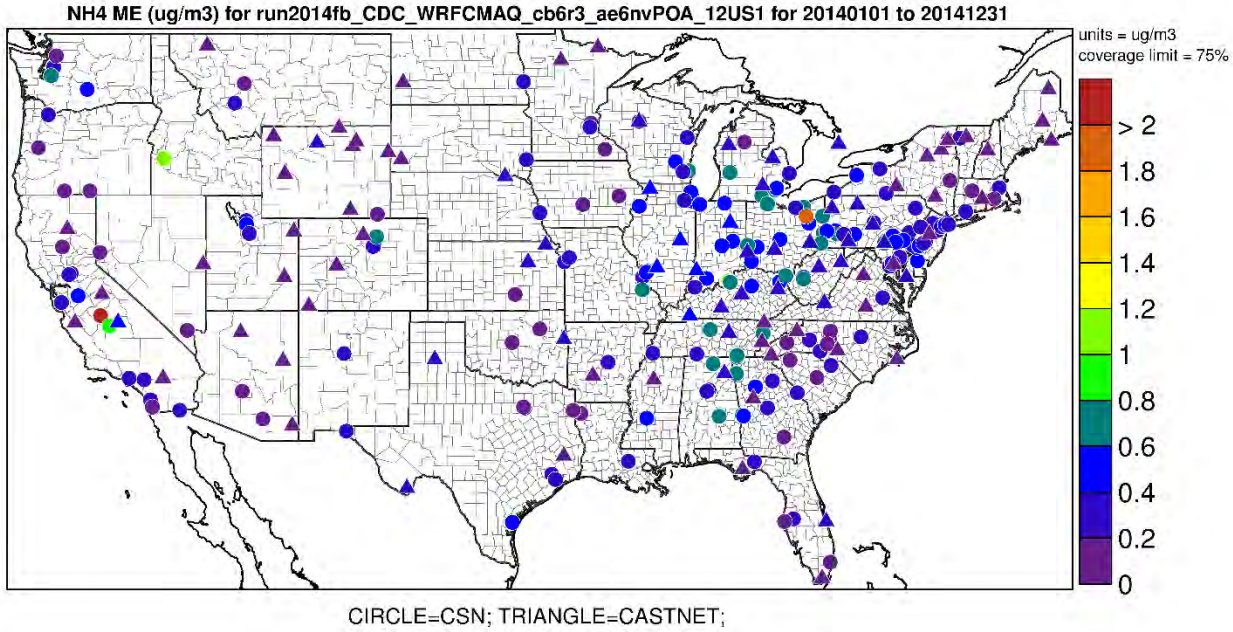



**Figure 4-20. Mean Error (µgm$^{-3}$) of annual ammonium at monitoring sites in the continental U.S. modeling domain.**

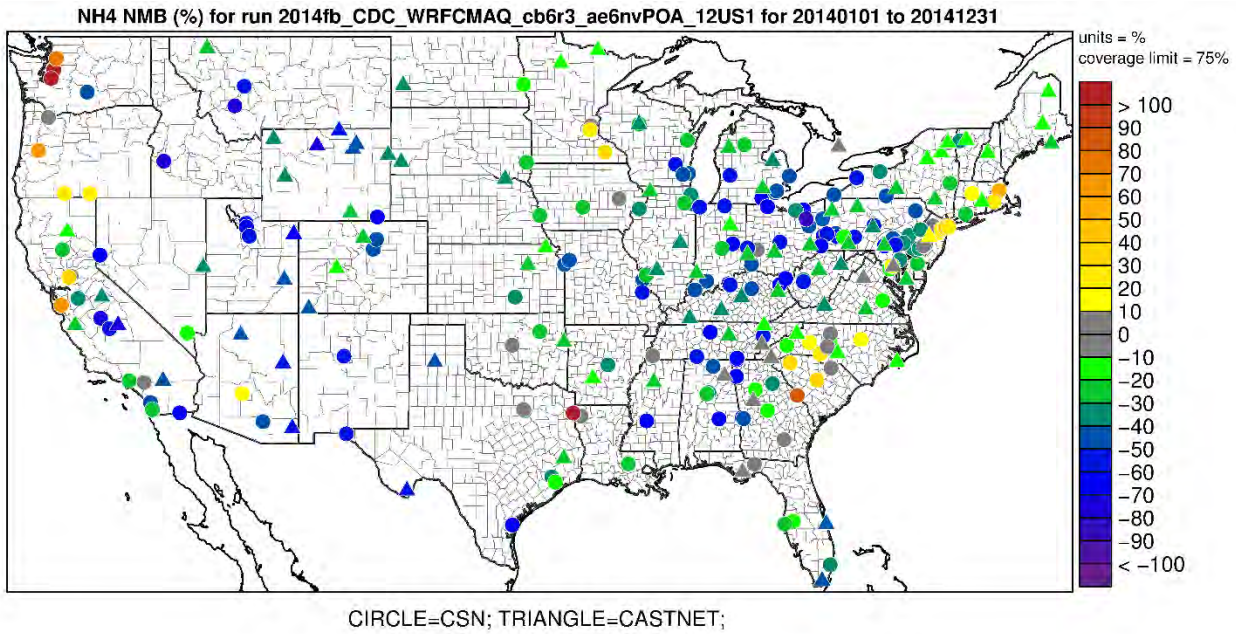



**Figure 4-21. Normalized Mean Bias (%) of annual ammonium at monitoring sites in the continental U.S. modeling domain.**

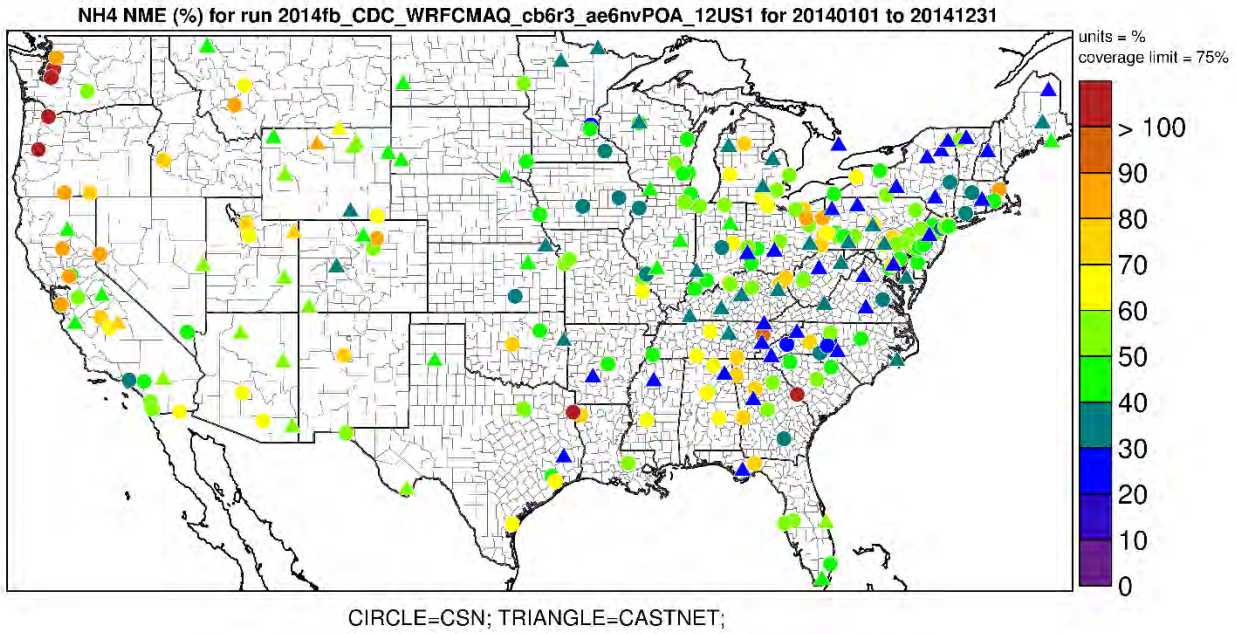



**Figure 4-22. Normalized Mean Error (%) of annual ammonium at monitoring sites in the continental U.S. modeling domain.**

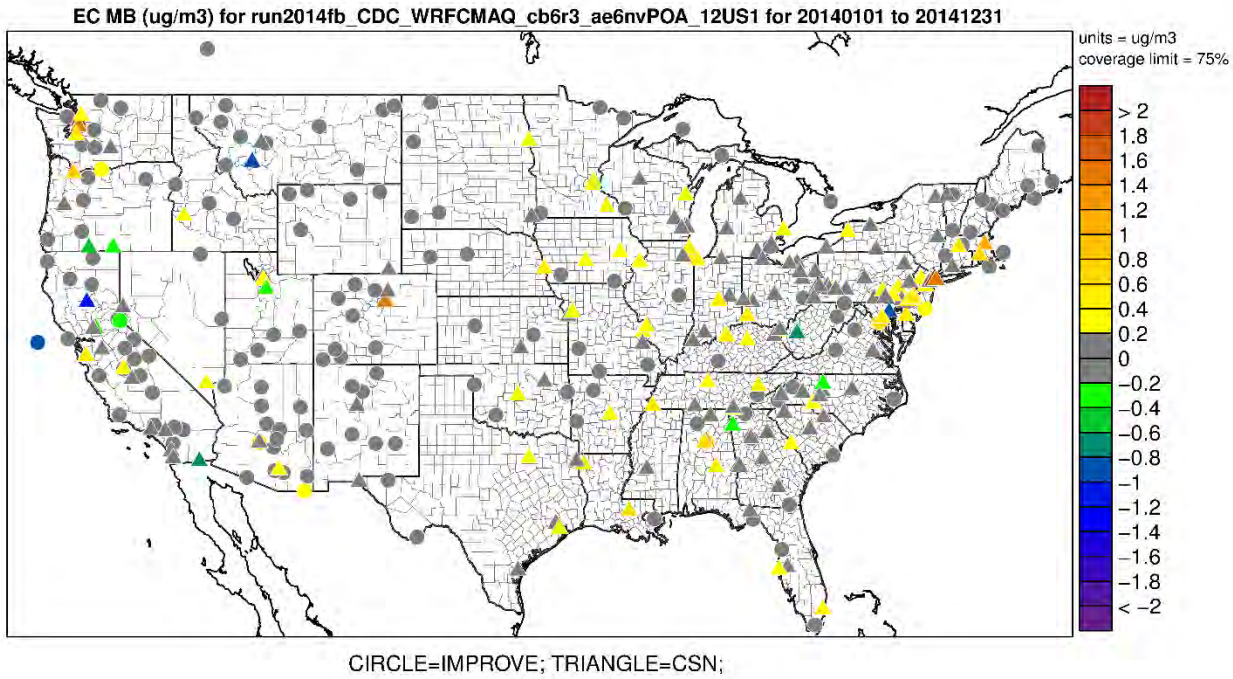



**Figure 4-23. Mean Bias ($\mu gm^{-3}$) of annual elemental carbon at monitoring sites in the continental U.S. modeling domain.**

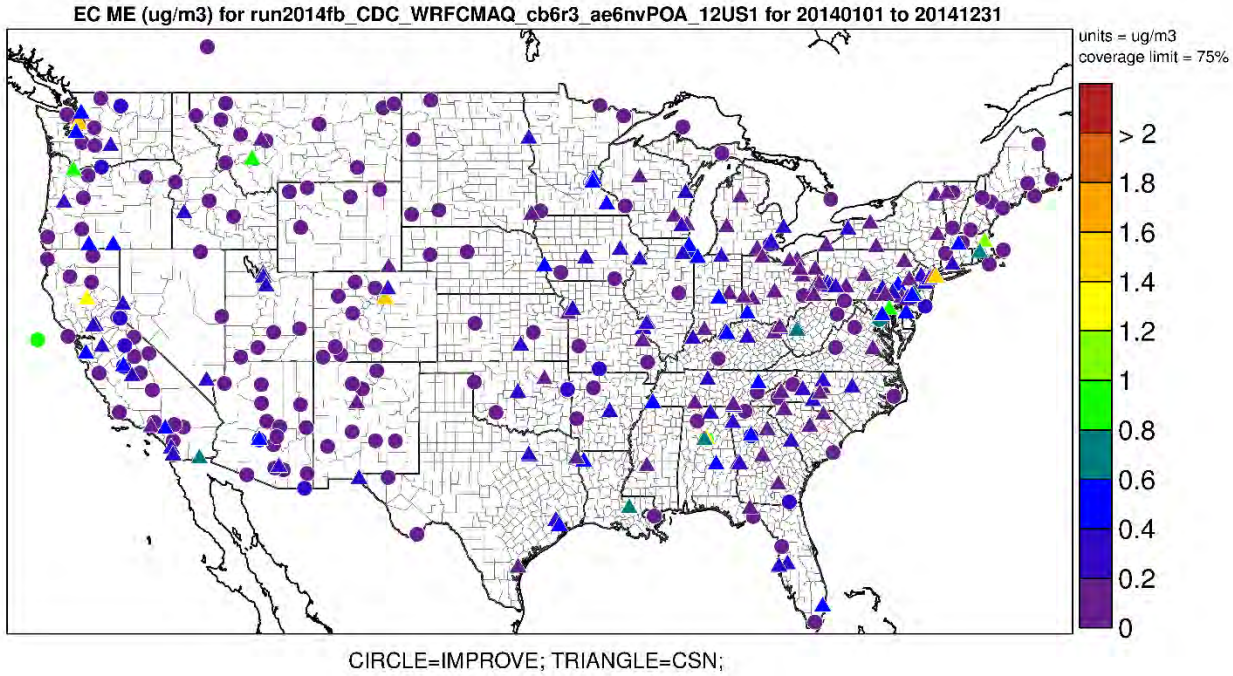



**Figure 4-24. Mean Error ($\mu gm^{-3}$) of annual elemental carbon at monitoring sites in the continental U.S. modeling domain.**

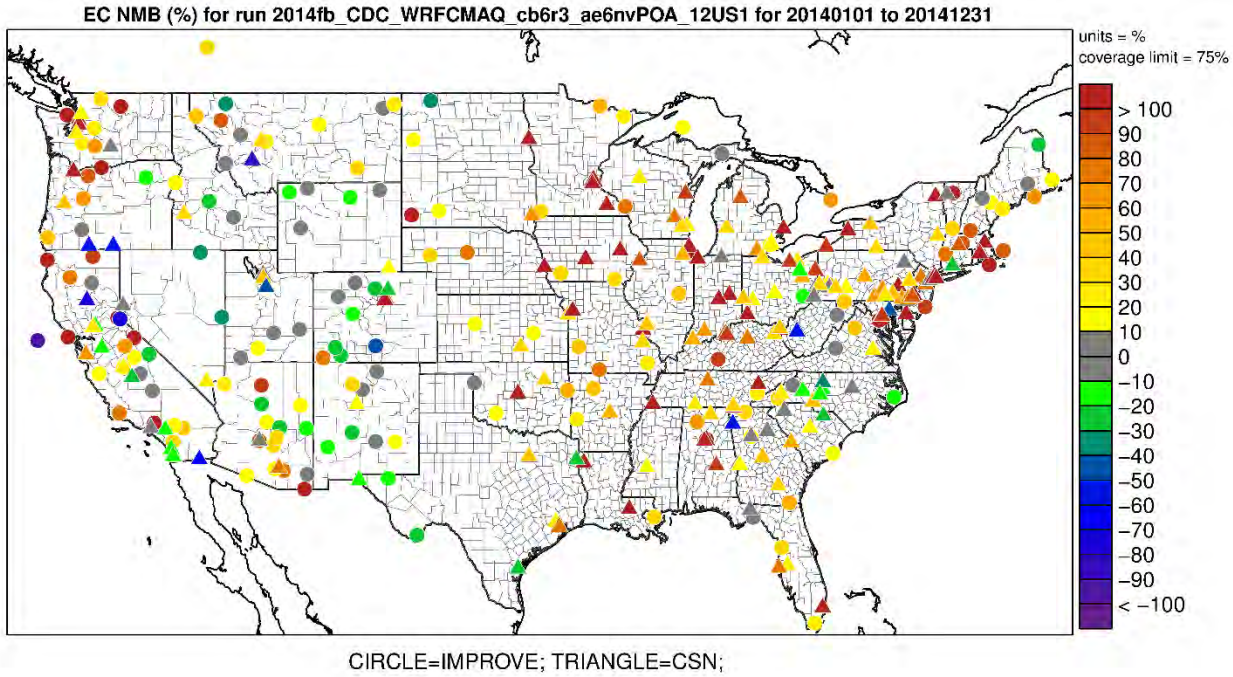



**Figure 4-25. Normalized Mean Bias (%) of annual elemental carbon at monitoring sites in the continental U.S. modeling domain.**

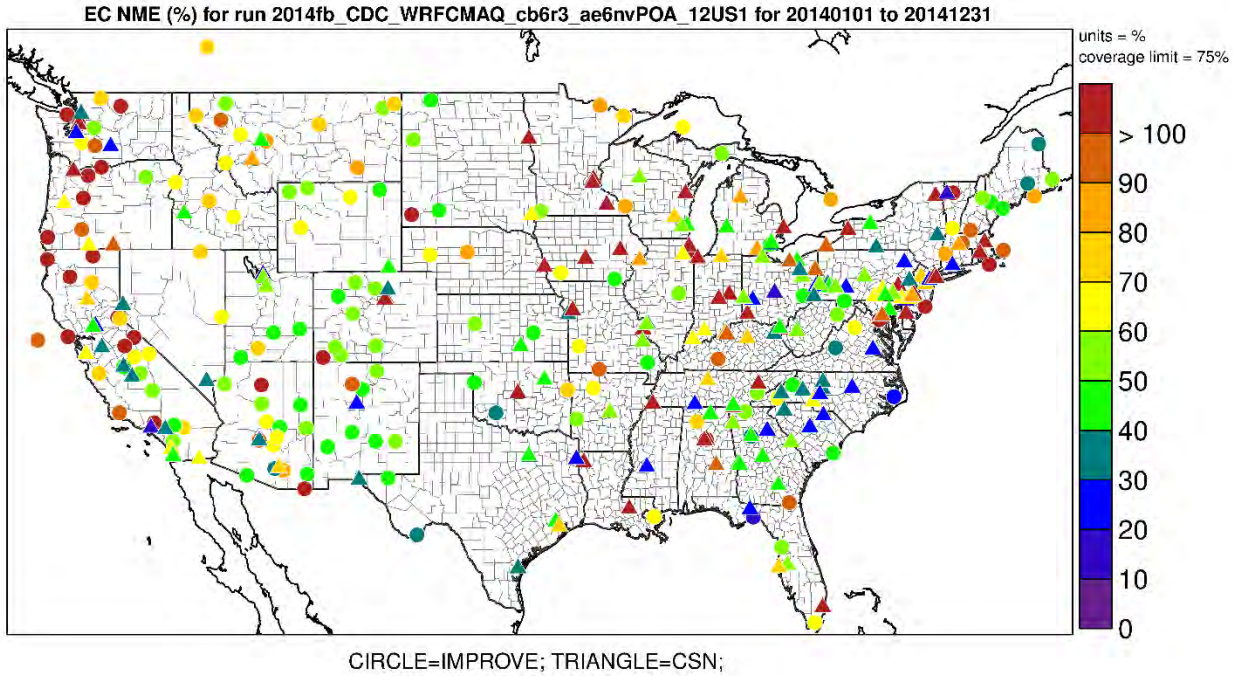



**Figure 4-26. Normalized Mean Error (%) of annual elemental carbon at monitoring sites in the continental U.S. modeling domain.**

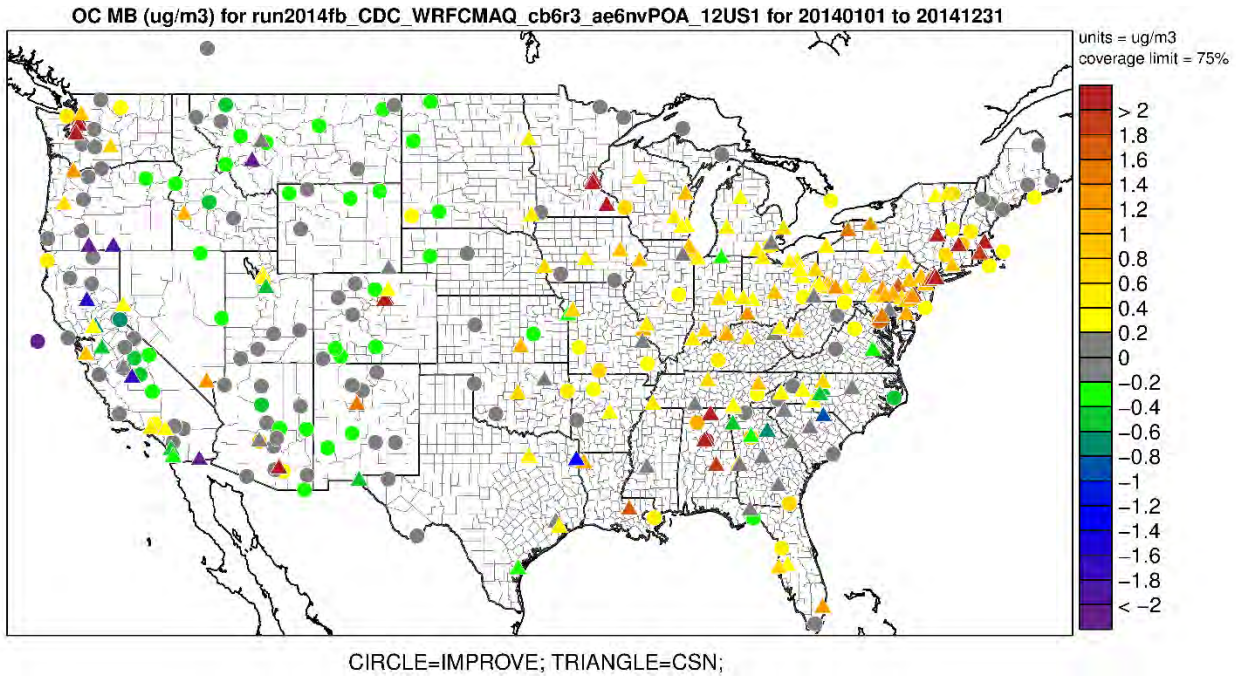



**Figure 4-27. Mean Bias ($\mu gm^{-3}$) of annual organic carbon at monitoring sites in the continental U.S. modeling domain.**

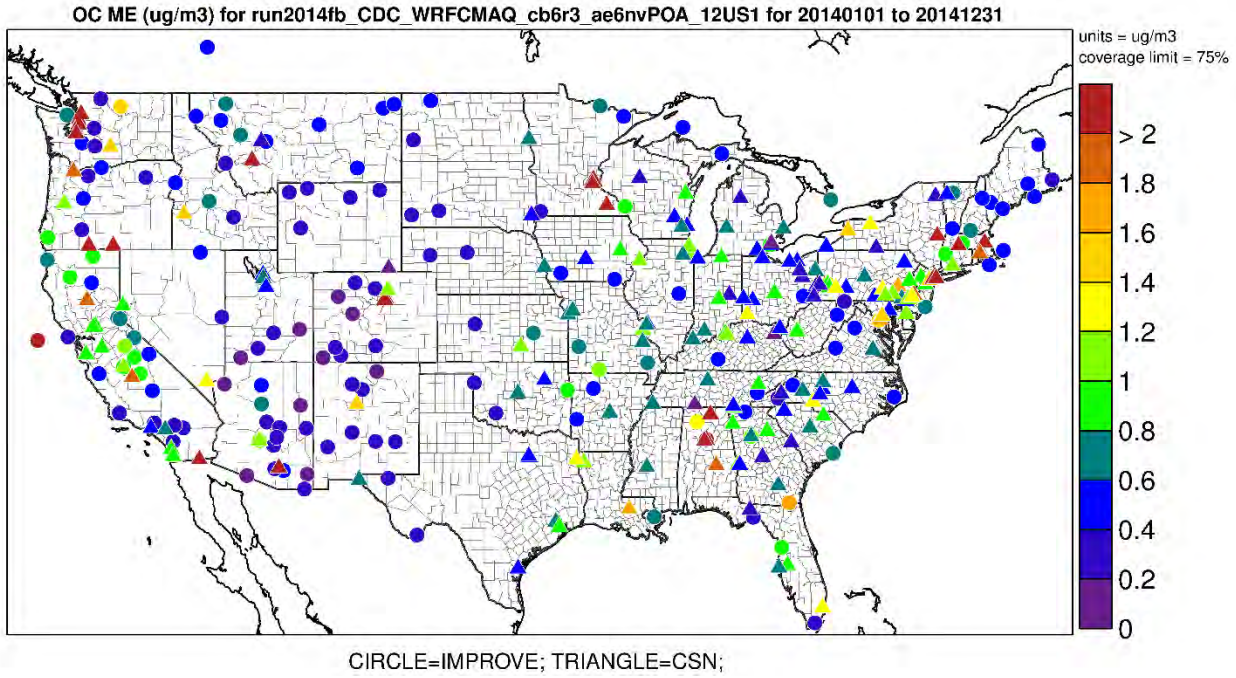



**Figure 4-28. Mean Error ($\mu gm^{-3}$) of annual organic carbon at monitoring sites in the continental U.S. modeling domain.**

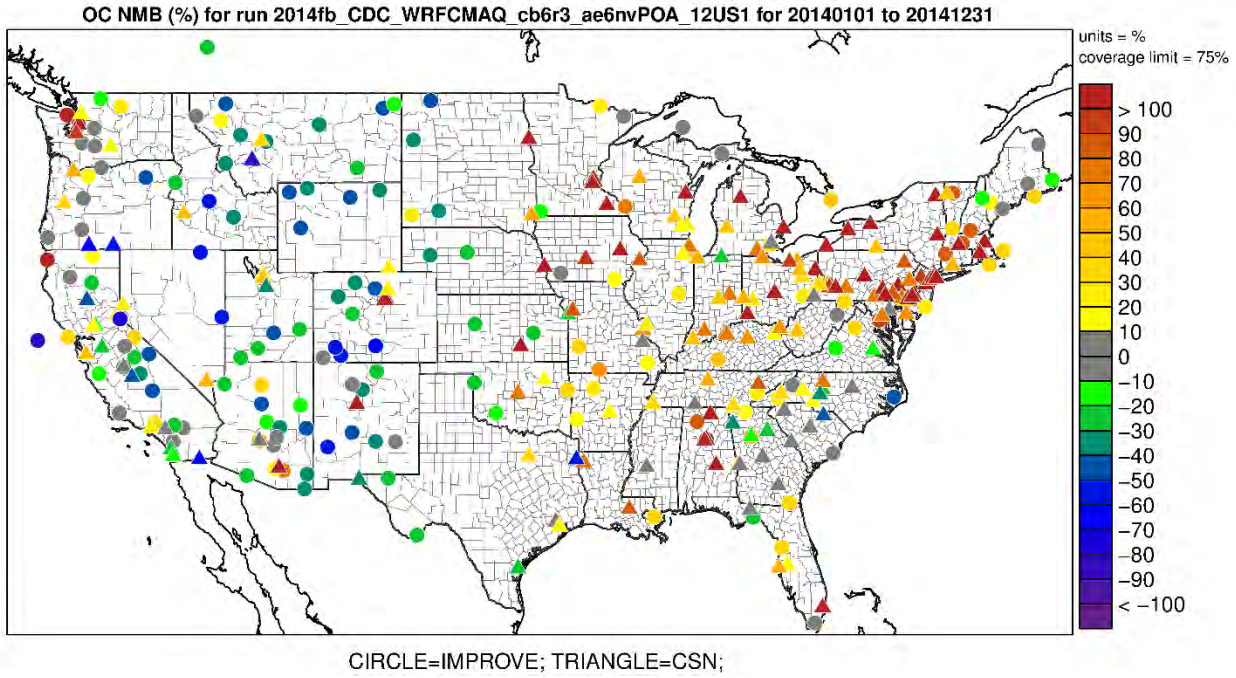



**Figure 4-29. Normalized Mean Bias (%) of annual organic carbon at monitoring sites in the continental U.S. modeling domain.**

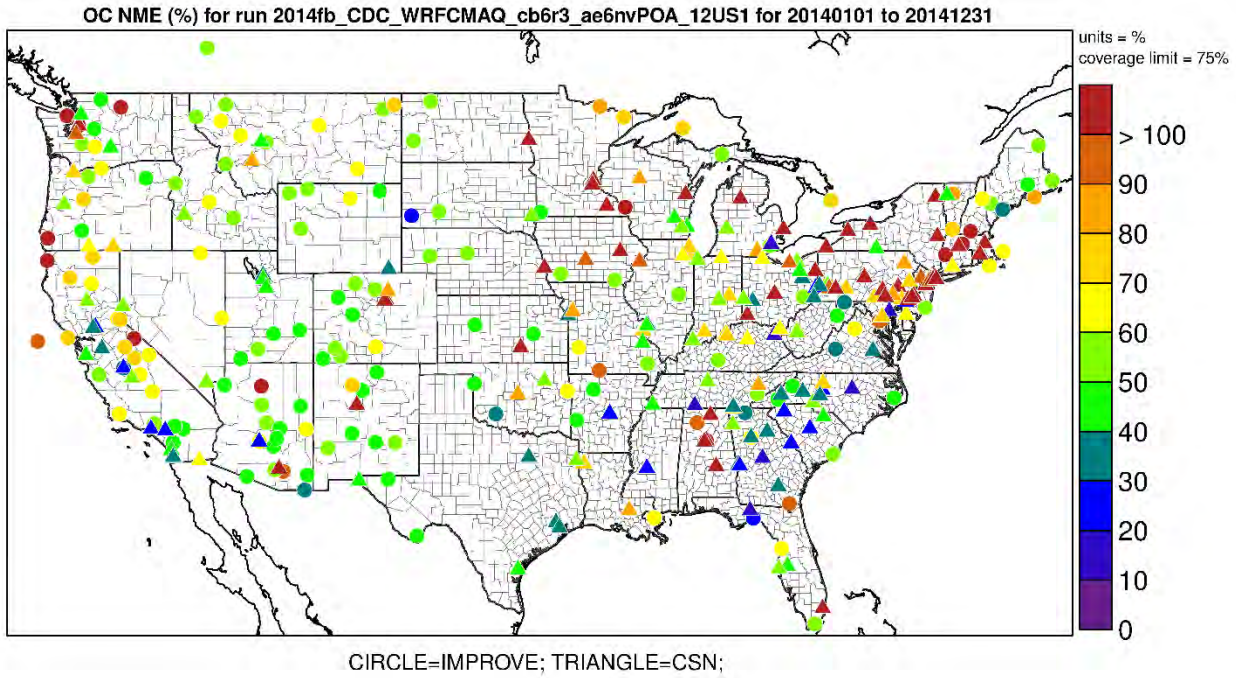



**Figure 4-30. Normalized Mean Bias (%) of annual organic carbon at monitoring sites in the continental U.S. modeling domain.**

# 5.0 Bayesian space-time downscaling fusion model (downscaler) - Derived Air Quality Estimates

## 5.1 Introduction

The need for greater spatial coverage of air pollution concentration estimates has grown in recent years as epidemiology and exposure studies that link air pollution concentrations to health effects have become more robust and as regulatory needs have increased. Direct measurement of concentrations is the ideal way of generating such data, but prohibitive logistics and costs limit the possible spatial coverage and temporal resolution of such a database. Numerical methods that extend the spatial coverage of existing air pollution networks with a high degree of confidence are thus a topic of current investigation by researchers. The downscaler model (DS) is the result of the latest research efforts by EPA for performing such predictions. DS utilizes both monitoring and CMAQ data as inputs, and attempts to take advantage of the measurement data's accuracy and CMAQ's spatial coverage to produce new spatial predictions. This chapter describes methods and results of the DS application that accompany this report, which utilized ozone and $PM_{2.5}$ data from AQS and CMAQ to produce predictions to continental U.S. 2010 census tract centroids for the year 2014.

## 5.2 Downscaler Model

DS develops a relationship between observed and modeled concentrations, and then uses that relationship to spatially predict what measurements would be at new locations in the spatial domain based on the input data. This process is separately applied for each time step (daily in this work) of data, and for each of the pollutants under study (ozone and $PM_{2.5}$). In its most general form, the model can be expressed in an equation similar to that of linear regression:

$$Y(s) = \tilde{\beta}_0(s) + \beta_1 \tilde{x}(s) + \varepsilon(s) \qquad \text{(Equation 1)}$$

Where:

*Y(s)* is the observed concentration at point *s*. Note that *Y(s)* could be expressed as $Y_t(s)$, where *t* indicates the model being fit at time *t* (in this case, *t=1,…,365* would represent day of the year.)
$\tilde{x}(s)$ is the point-level regressor based on the CMAQ concentration at point *s*. This value is a weighted average of both the gridcell containing the monitor and neighboring gridcells.
$\tilde{\beta}_0(s)$ is the intercept, where $\tilde{\beta}_0(s) = \beta_0 + \beta_0(s)$ is composed of both a global component $\beta_0$ and a local component $\beta_0(s)$ that is modeled as a mean-zero Gaussian Process with exponential decay
$\beta_1$ is the global slope; local components of the slope are contained in the $\tilde{x}(s)$ term.
$\varepsilon(s)$ is the model error.

DS has additional properties that differentiate it from linear regression:

1) Rather than just finding a single optimal solution to Equation 1, DS uses a Bayesian approach so that uncertainties can be generated along with each concentration prediction. This involves drawing random

samples of model parameters from built-in "prior" distributions and assessing their fit on the data on the order of thousands of times. After each iteration, properties of the prior distributions are adjusted to try to improve the fit of the next iteration. The resulting collection of $\tilde{\beta}_0$ and $\beta_1$ values at each space-time point are the "posterior" distributions, and the means and standard distributions of these are used to predict concentrations and associated uncertainties at new spatial points.

2) The model is "hierarchical" in structure, meaning that the top level parameters in Equation 1 (ie $\tilde{\beta}_0(s)$, $\beta_1$, $\tilde{x}(s)$) are actually defined in terms of further parameters and sub-parameters in the DS code. For example, the overall slope and intercept is defined to be the sum of a global (one value for the entire spatial domain) and local (values specific to each spatial point) component. This gives more flexibility in fitting a model to the data to optimize the fit (i.e. minimize $\varepsilon(s)$).

Further information about the development and inner workings of the current version of DS can be found in Berrocal, Gelfand and Holland (2012)38 and references therein. The DS outputs that accompany this report are described below, along with some additional analyses that include assessing the accuracy of the DS predictions. Results are then summarized, and caveats are provided for interpreting them in the context of air quality management activities.

## 5.3 Downscaler Concentration Predictions

In this application, DS was used to predict daily concentration and associated uncertainty values at the 2014 US census tract centroids across the continental U.S. using 2014 measurement and CMAQ data as inputs. For ozone, the concentration unit is the daily maximum 8-hour average in ppb and for $PM_{2.5}$ the concentration unit is the 24-hour average in $\mu g/m^3$.

### *5.3.1 Summary of 8-hour Ozone Results*

Figure 5-1 summarizes the AQS, CMAQ and DS ozone data over the year 2014. It shows the 4$^{th}$ max daily maximum 8-hour average ozone for AQS observations, CMAQ model predictions and DS model results. The DS model estimated that for 2014, about 23% of the US Census tracts (16815 out of 72283) experienced at least one day with an ozone value above the NAAQS of 75 ppb.

38 Berrocal, V., Gelfand, A., and D. Holland. Space-Time Data Fusion Under Error in Computer Model Output: An Application to Modeling Air Quality. *Biometrics.* 2012. September ; 68(3): 837–848. doi:10.1111/j.1541-0420.2011.01725.x

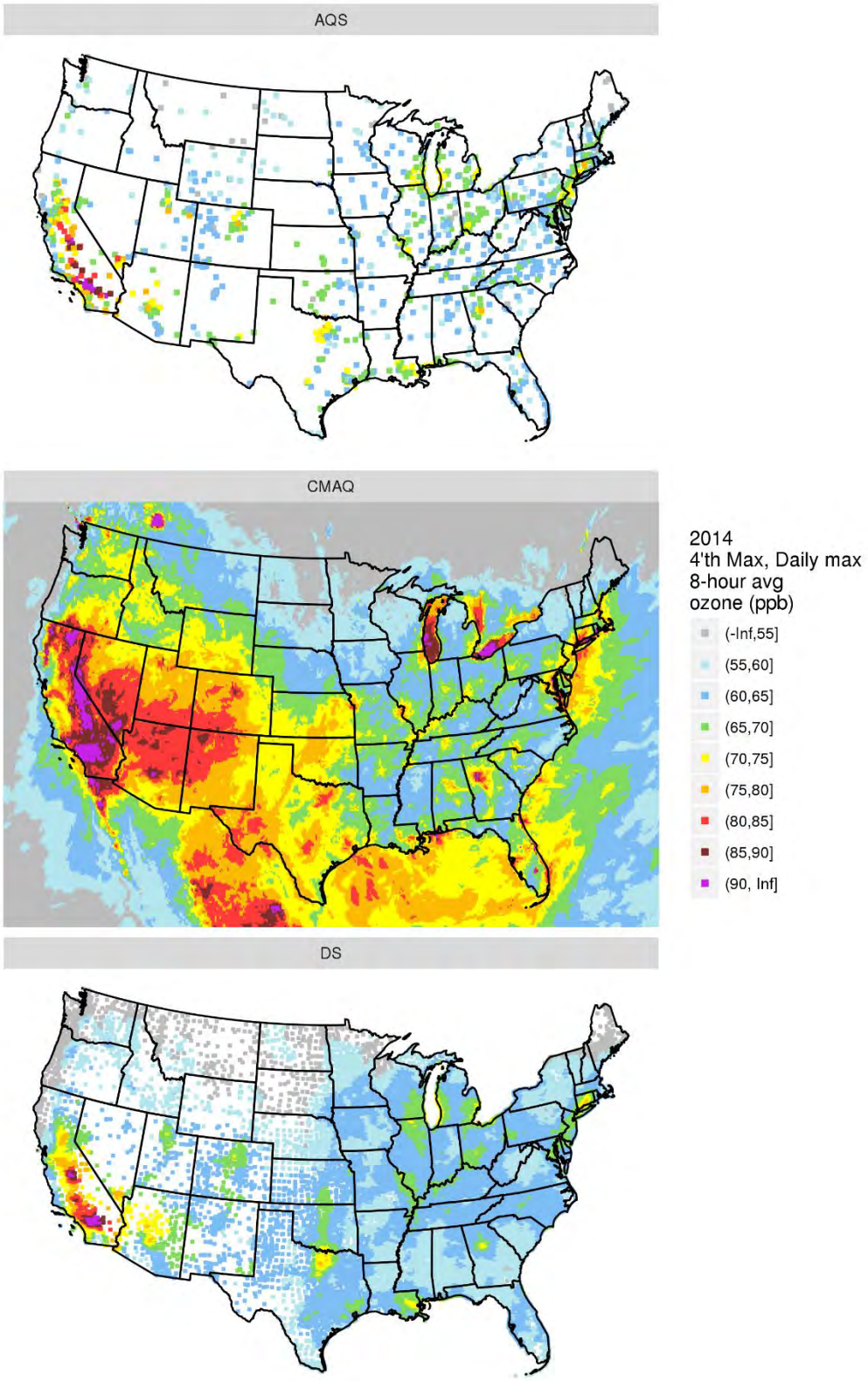



**Figure 5-1. Annual 4th max (daily max 8-hour ozone concentrations) derived from AQS, CMAQ and DS data.**

### *5.3.2 Summary of $PM_{2.5}$ Results*

Figures 5-2 and 5-3 summarize the AQS, CMAQ and DS PM2.5 data over the year 2014. Figure 5-2 shows annual means and Figure 5-3 shows 98$^{th}$percentiles of 24-hour PM2.5 concentrations for AQS observations, CMAQ model predictions and DS model results. The DS model estimated that for 2014 about 34% of the US Census tracts (24328 out of 72283) experienced at least one day with a PM2.5 value above the 24-hour NAAQS of 35 $\mu g/m^3$.

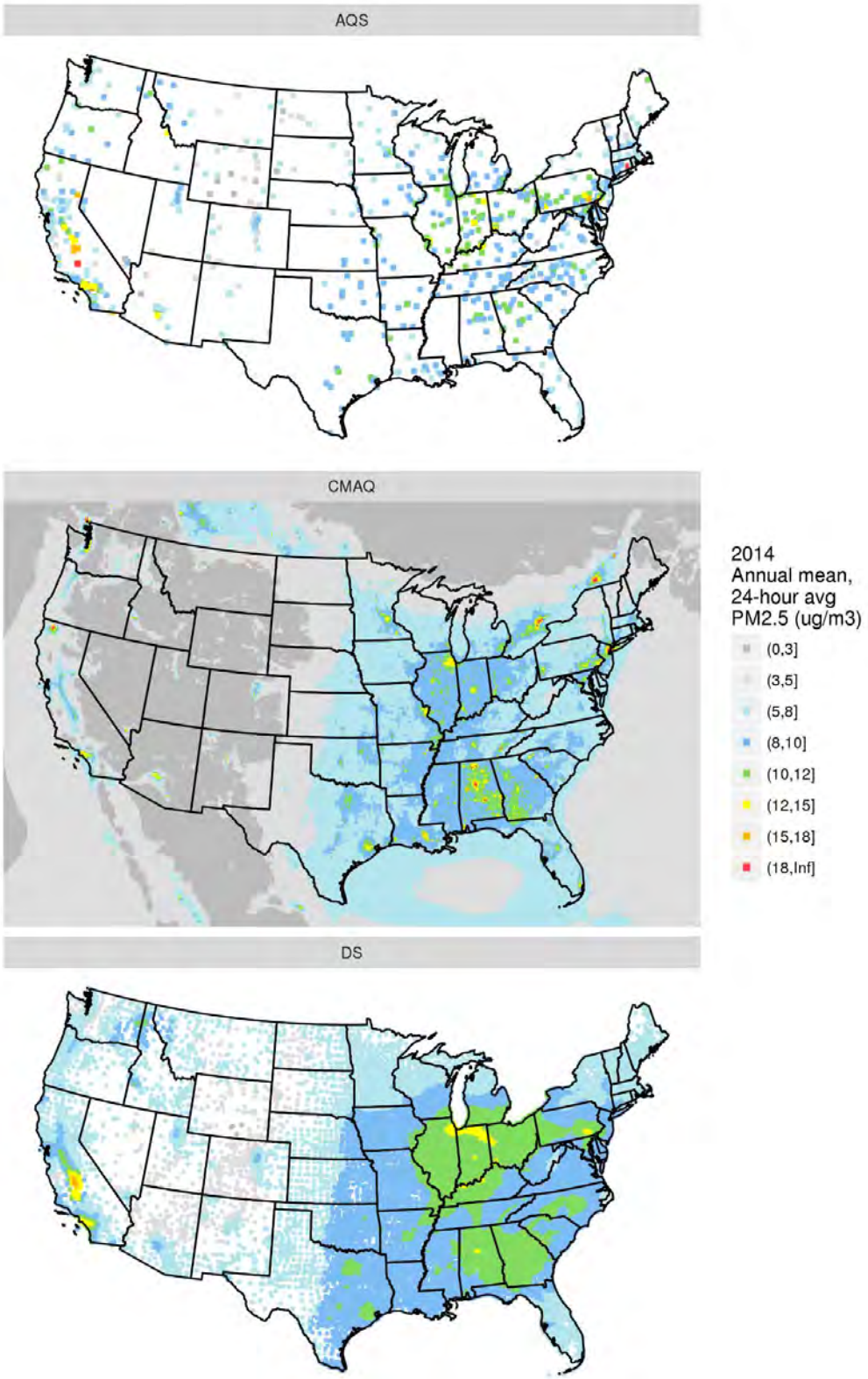



**Figure 5-2. Annual mean $PM_{2.5}$ concentrations derived from AQS, CMAQ and DS data.**

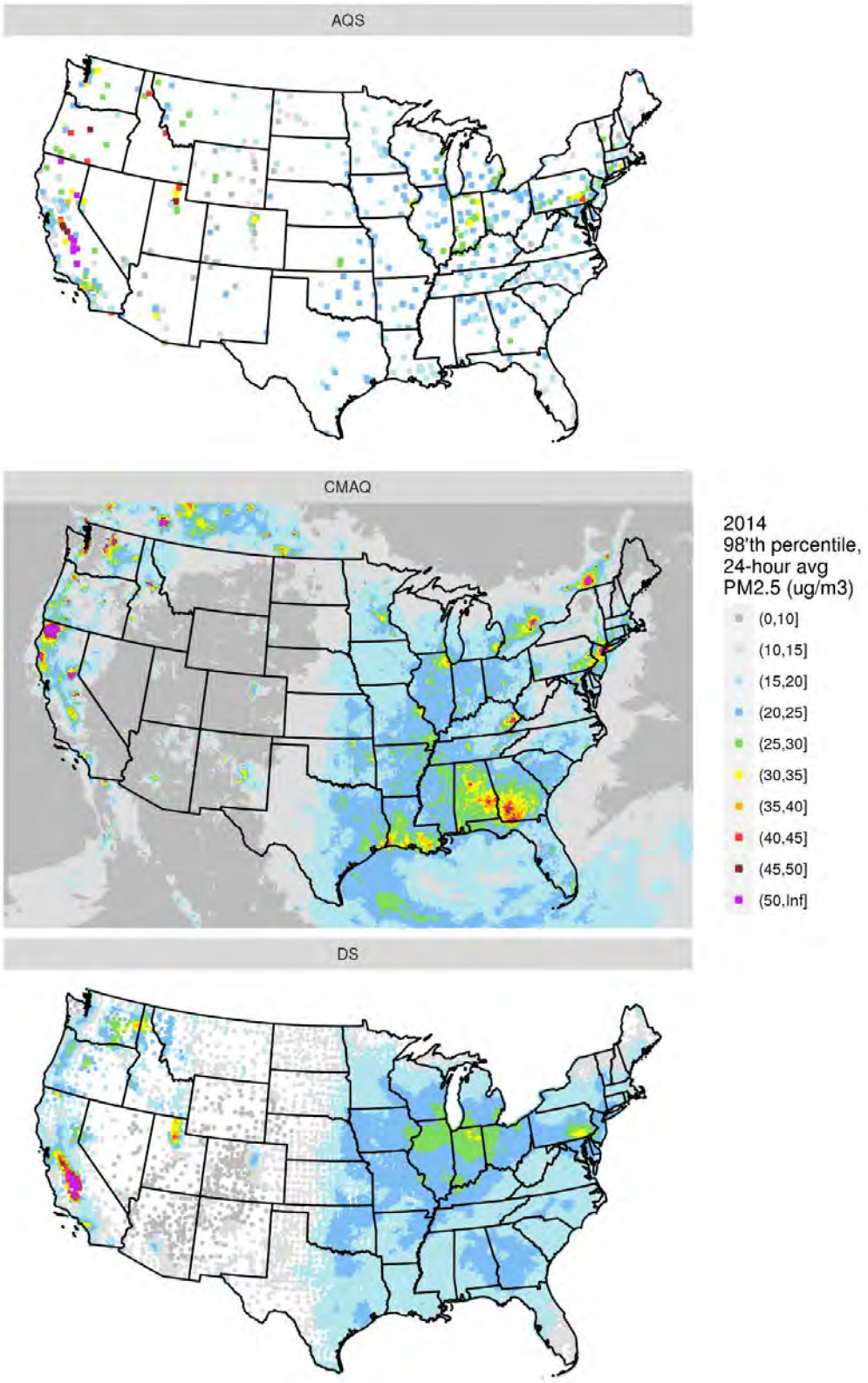



**Figure 5-3. 98th percentile 24-hour average $PM_{2.5}$ concentrations derived from AQS, CMAQ and DS data.**

## 5.4 Downscaler Uncertainties

### *5.4.1 Standard Errors*

As mentioned above, the DS model works by drawing random samples from built-in distributions during its parameter estimation. The standard errors associated with each of these populations provide a measure of uncertainty associated with each concentration prediction. Figure 5-4 shows the percent errors resulting from dividing the DS standard errors by the associated DS prediction. The black dots on the maps show the location of EPA sampling network monitors whose data was input to DS via the AQS datasets (Chapter 2). The maps show that, in general, errors are relatively smaller in regions with more densely situation monitors (ie the eastern US), and larger in regions with more sparse monitoring networks (ie western states). These standard errors could potentially be used to estimate the probability of an exceedance for a given point estimate of a pollutant concentration.

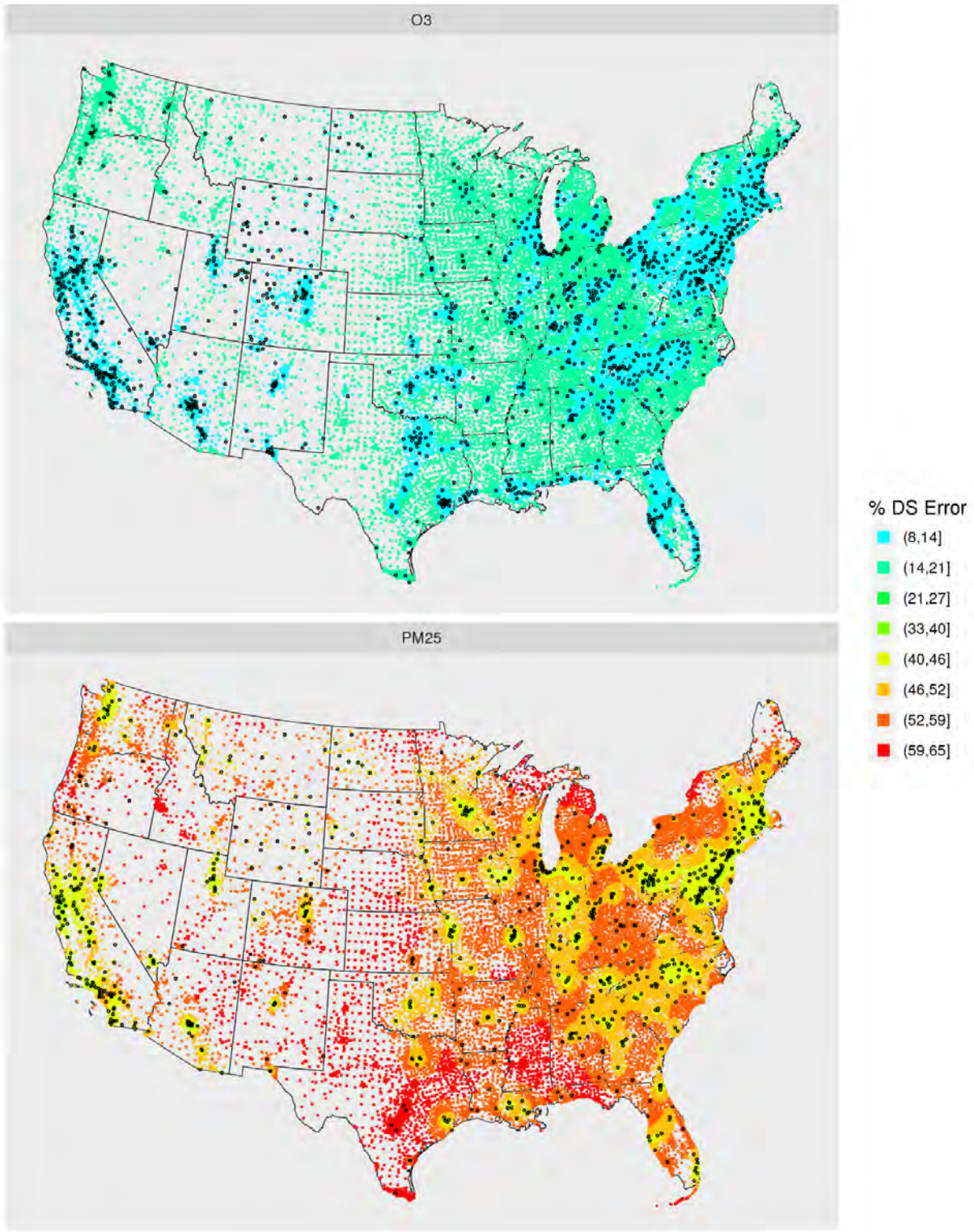



**Figure 5-4. Annual mean relative errors (standard errors divided by predictions) from the DS 2014 runs. The black dots show the locations of monitors that generated the AQS data used as input to the DS model.**

### *5.4.2 Cross Validation*

To check the quality of its spatial predictions, DS can be set to perform "cross-validation" (CV), which involves leaving a subset of AQS data out of the model run and predicting the concentrations of those left out points. The predicted values are then compared to the actual left-out values to generate statistics that provide an indicator of the predictive ability. In the DS runs associated with this report, 10% of the data was chosen randomly by the DS model to be used for the CV process. The resulting CV statistics are shown below in Table 5-1.

| Pollutant | # Monitors | Mean Bias | RMSE | Mean Coverage |
|---|---|---|---|---|
| PM2.5 | 943 | 0.286 | 3.42 | 0.95 |
| O3 | 1299 | -0.0162 | 4.50 | 0.96 |

**Table 5-1. Cross-validation statistics associated with the 2014 DS runs.**

The statistics indicated by the columns of Table 5-1 are as follows:

- Mean Bias: The bias of each prediction is the DS prediction minus the AQS value. This column is the mean of all biases across the CV cases.

- Root Mean Squared Error (RMSE): The bias is squared for each CV prediction, then the square root of the mean of all squared biases across all CV predictions is obtained.

- Mean Coverage: A value of 1 is assigned if the measured AQS value lies in the 95% confidence interval of the DS prediction (the DS prediction +/- the DS standard error), and 0 otherwise. This column is the mean of all those 0's and 1's.

## 5.5 Summary and Conclusions

The results presented in this report are from an application of the DS fusion model for characterizing national air quality for Ozone and $PM_{2.5}$. DS provided spatial predictions of daily ozone and $PM_{2.5}$ at 2010 U.S. census tract centroids by utilizing monitoring data and CMAQ output for 2014. Large-scale spatial and temporal patterns of concentration predictions are generally consistent with those seen in ambient monitoring data. Both Ozone and $PM_{2.5}$ were predicted with lower error in the eastern versus the western U.S., presumably due to the greater monitoring density in the east.

An additional caution that warrants mentioning is related to the capability of DS to provide predictions at multiple spatial points within a single CMAQ gridcell. Care needs to be taken not to over-interpret any within-gridcell gradients that might be produced by a user. Fine-scale emission sources in CMAQ are diluted into the gridcell averages, but a given source within a gridcell might or might not affect every spatial point contained therein equally. Therefore DS-generated fine-scale gradients are not expected to represent actual fine-scale atmospheric concentration gradients, unless possibly where multiple monitors are present in the gridcell.

# Appendix A - Acronyms

**Acronyms**

| | |
|---|---|
| ARW | Advanced Research WRF core model |
| BEIS | Biogenic Emissions Inventory System |
| BlueSky | Emissions modeling framework |
| CAIR | Clean Air Interstate Rule |
| CAMD | EPA's Clean Air Markets Division |
| CAP | Criteria Air Pollutant |
| CAR | Conditional Auto Regressive spatial covariance structure (model) |
| CARB | California Air Resources Board |
| CEM | Continuous Emissions Monitoring |
| CHIEF | Clearinghouse for Inventories and Emissions Factors |
| CMAQ | Community Multiscale Air Quality model |
| CMV | Commercial marine vessel |
| CO | Carbon monoxide |
| CSN | Chemical Speciation Network |
| DQO | Data Quality Objectives |
| EGU | Electric Generating Units |
| Emission Inventory | Listing of elements contributing to atmospheric release of pollutant substances |
| EPA | Environmental Protection Agency |
| EMFAC | Emission Factor (California's onroad mobile model) |
| FAA | Federal Aviation Administration |
| FDDA | Four Dimensional Data Assimilation |
| FIPS | Federal Information Processing Standards |
| HAP | Hazardous Air Pollutant |
| HMS | Hazard Mapping System |
| ICS-209 | Incident Status Summary form |
| IPM | Integrated Planning Model |
| ITN | Itinerant |
| LSM | Land Surface Model |
| MOBILE | OTAQ's model for estimation of onroad mobile emissions factors |
| MODIS | Moderate Resolution Imaging Spectroradiometer |
| MOVES | Motor Vehicle Emission Simulator |
| NEEDS | National Electric Energy Database System |
| NEI | National Emission Inventory |
| NERL | National Exposure Research Laboratory |
| NESHAP | National Emission Standards for Hazardous Air Pollutants |
| NH | Ammonia |
| NMIM | National Mobile Inventory Model |
| NONROAD | OTAQ's model for estimation of nonroad mobile emissions |
| NO | Nitrogen oxides |
| OAQPS | EPA's Office of Air Quality Planning and Standards |

| | |
|---|---|
| OAR | EPA's Office of Air and Radiation |
| ORD | EPA's Office of Research and Development |
| ORIS | Office of Regulatory Information Systems (code) - is a 4 or 5 digit number assigned by the Department of Energy's (DOE) Energy Information Agency (EIA) to facilities that generate electricity |
| ORL | One Record per Line |
| OTAQ | EPA's Office of Transportation and Air Quality |
| PAH | Polycyclic Aromatic Hydrocarbon |
| 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 |
| PMc | Particulate matter greater than 2.5 microns and less than 10 microns |
| Prescribed Fire | Intentionally set fire to clear vegetation |
| RIA | Regulatory Impact Analysis |
| RPO | Regional Planning Organization |
| RRTM | Rapid Radiative Transfer Model |
| SCC | Source Classification Code |
| SMARTFIRE | Satellite Mapping Automatic Reanalysis Tool for Fire Incident Reconciliation |
| SMOKE | Sparse Matrix Operator Kernel Emissions |
| TCEQ | Texas Commission on Environmental Quality |
| TSD | Technical support document |
| VOC | Volatile organic compounds |
| VMT | Vehicle miles traveled |
| Wildfire | Uncontrolled forest fire |
| WRAP | Western Regional Air Partnership |
| WRF | Weather Research and Forecasting Model |

| | | |
|---|---|---|
| United States<br>Environmental Protection<br>Agency | Office of Air Quality Planning and Standards<br>Air Quality Assessment Division<br>Research Triangle Park, NC | Publication No. EPA-454/R-18-008<br>October 2018 |