Bayesian Space-time Downscaling Fusion Model (Downscaler) - Derived Estimates of Air Quality for 2018

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1.0   Introduction

This report describes estimates of daily ozone (maximum 8-hour average) and fine particulate matter (PM$_{2.5}$) (24-hour average) concentrations throughout the contiguous United States during the 2018 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 DS 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 PM$_{2.5}$.

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] approach 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 (https://www.cdc.gov/nceh/tracking/). 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 variety of sources and to examine, analyze and interpret those data based on their spatial and temporal characteristics.

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[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.

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 EPA, 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 EPA shall not be held liable for improper or incorrect use of the data described and/or contained herein.

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

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

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[2] The original HHS and EPA MOU is available at https://www.cdc.gov/nceh/tracking/pdfs/epa_mou_2007.pdf.

- 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 U.S. census tract centroid locations within the contiguous U.S.

- Appendix A provides a description of acronyms used in this report.

- Appendix B is a separate spreadsheet that shows emissions totals for the modeling domain and for each emissions modeling sector (see Section 3 for more details).

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 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 ozone designations, go to https://www.epa.gov/ozone-designations and for PM designations, go to 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 CAA 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 National Ambient Air Quality Standards

Form of the Standard (parts per million, ppm)	1997	2008	2015
Annual 4th highest daily max 8-hour average, averaged over three years	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 sources.[3] 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 ($PM_{10-2.5}$) 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.

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[3] 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 98th 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$_{2.5}$ National Ambient Air Quality Standards

Form of the Standard (micrograms per cubic meter, μg/m^3)	1997	2006	2012
Annual mean of 24-hour averages, averaged over 3 years	15.0	15.0	12.0
98th percentile of 24-hour averages, averaged over 3 years	65	35	35

2.2   Ambient Air Quality Monitoring in the United States

2.2.1   Monitoring Networks

The CAA (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 PM2.5 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 2019, approximately 40 percent of the U.S. population was living within 10 kilometers of ozone and PM$_{2.5}$ monitoring sites. Highly populated areas in the eastern U.S. and California are well covered by both ozone and PM$_{2.5}$ monitoring network (Figure 2-1).

Distance to the Nearest Ozone Monitor
- < 10 km (30,224 tracts / 132 million people)
- 10 km - 25 km (25,065 tracts / 120 million people)
- 25 km - 50 km (10,369 tracts / 45.7 million people)
- 50 km - 75 km (3,935 tracts / 14.6 million people)
- 75 km - 100 km (1,864 tracts / 6.9 million people)
- 100 km - 150 km (1512 tracts / 5.5 million people)
- 150 km < (712 tracts / 2.7 million people)

Distance to the Nearest PM 2.5 Monitor
- < 10 km (30,904 tracts / 130 million people)
- 10 km - 25 km (20,910 tracts / 102.5 million people)
- 25 km - 50 km (11,643 tracts / 53.6 million people)
- 50 km - 75 km (5,638 tracts / 23.5 million)
- 75 km - 100 km (2,309 tracts / 9.1 million people)
- 100 km - 150 km (1,771 tracts / 6.9 million people)
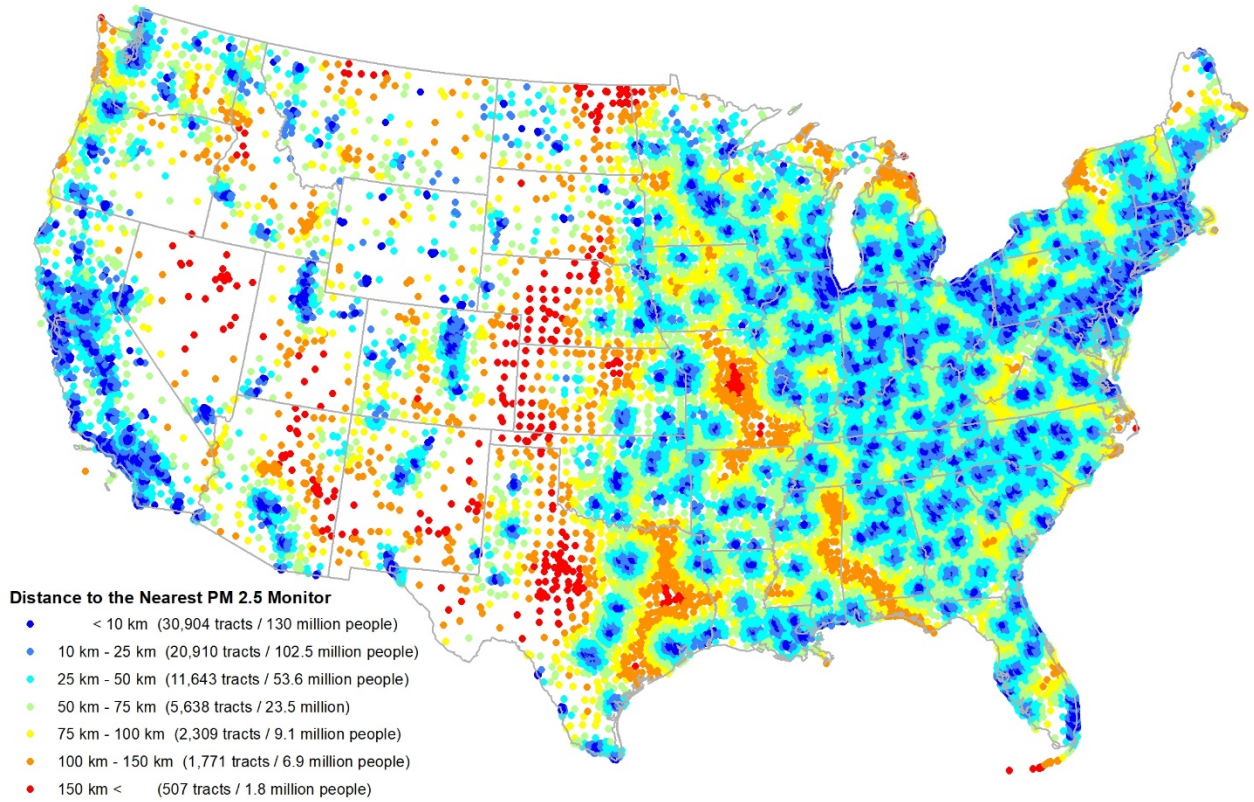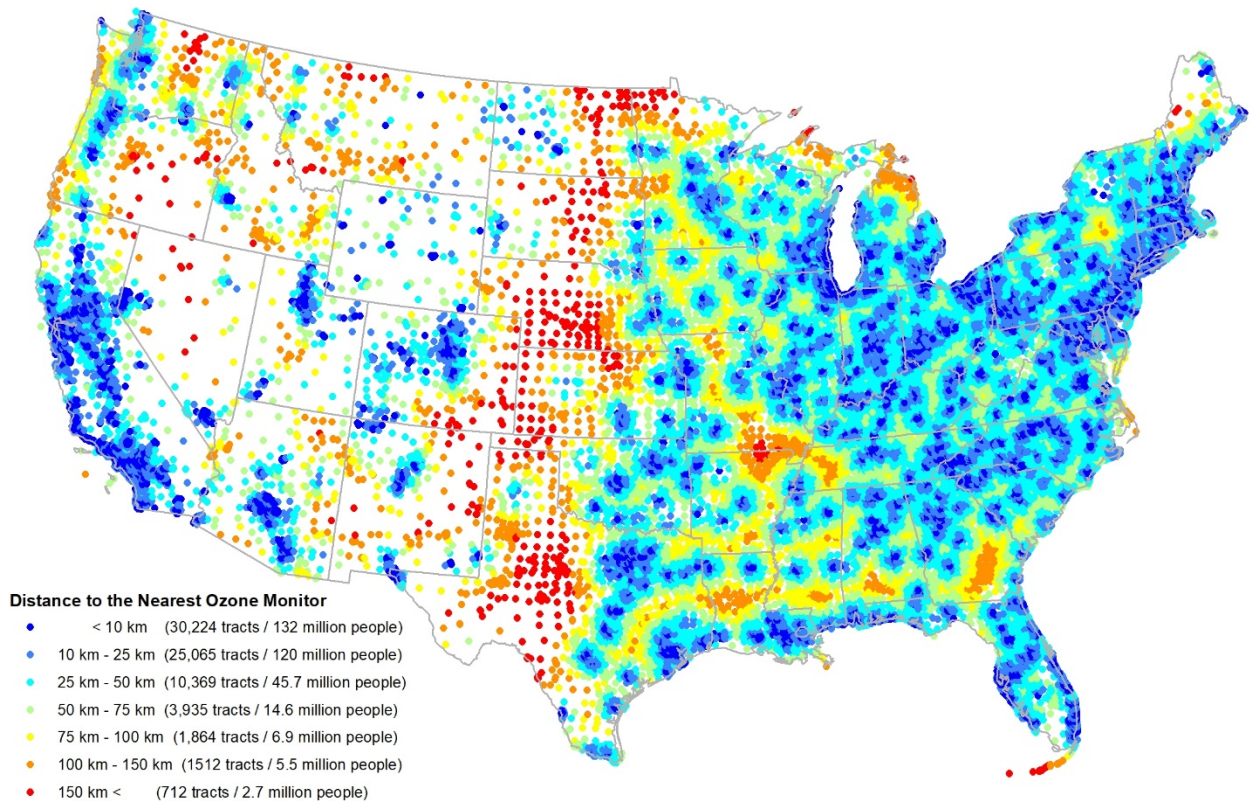- 150 km < (507 tracts / 1.8 million people)

Figure 2-1. Distances from U.S. Census Tract centroids to the nearest monitoring site, 2019.

In summary, state and local agencies and tribes implement a quality-assured monitoring network to measure air quality across the U.S. The 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 OAQPS 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 EPHT activities.

The advantage of using ambient data from EPA monitoring networks for comparison 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.[4] 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 samples. However, in recent years, continuous monitors have become available which can automatically collect, analyze, and report $PM_{2.5}$ measurements on an hourly

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[4] 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.

basis. 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 Federal Equivalent Methods (FEM).

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 workplace 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 CMAQ 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[5] is an example of an earlier approach for merging air quality monitor data with CMAQ model predictions. DS 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 DS. 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 2-3. 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.	Data are available through state agencies and EPA's AQS. EPA and CDC developed an interagency agreement, where EPA provides air quality data along with statistically combined AQS and CMAQ 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, Generate hypothesis for further research, and 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.

Table 2-4. 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 FRM)
• Number of days with maximum ozone concentration over the NAAQS (or other relevant benchmarks (by county and MSA)   • 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).   • Percent of population exceeding annual $PM_{2.5}$ NAAQS (by state).   • Percent of days with $PM_{2.5}$ concentration over the daily NAAQS (or other relevant benchmarks (by county and MSA)   • 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 EPA's 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 representing the year 2018 for this project that was based on the 2017 National Emissions Inventory (NEI) as well as inventories developed for EPA's Air Quality Time Series (EQUATES) project (Foley, 2020). This section provides a summary of the emissions inventory and emissions modeling techniques applied to Criteria Air Pollutants (CAPs) and specific Hazardous Air Pollutants (HAPs). 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 CMAQ model (https://www.epa.gov/cmaq) was used to model ozone (O_3) and particulate matter (PM) for this project. CMAQ requires hourly 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 mechanism version 6 (CB6) with chlorine chemistry within CMAQ allows for explicit treatment of the VOC HAPs including naphthalene, benzene, acetaldehyde, formaldehyde and methanol (NBAFM) and also includes hydrochloric acid (HCl) and chlorine (Cl).

The effort to create the emission inputs for this study included development of emission inventories for input to a 2018 modeling case, along with the application of emissions modeling tools to convert the inventories into the format and resolution needed by CMAQ. Year-specific emissions were used for fires, biogenic sources, fertilizer, point sources, and onroad and nonroad mobile sources. Where available, continuous emission monitoring system (CEMS) data were used for electric generating unit (EGU) emissions. The remaining emission inventories were adjusted to represent 2018, primarily using 2017-specific emissions as a starting point. 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 4.8.1 was used to create CMAQ-ready emissions files for a 12-km national grid. Additional information about SMOKE is available from http://www.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, which are based on the January 2021 version of the 2017 NEI along with the point source inventory for 2018 along with other 2018-specific data. 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 point source CAPs, the NEI data are largely compiled from data submitted by state, local and tribal (S/L/T) agencies. States are encouraged to submit inputs to emissions computation tools for many nonpoint categories, which EPA then uses to compute the emissions. 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 2017 NEI Technical Support Document describes in detail the development of the 2017 emission inventories and is available at https://www.epa.gov/air-emissions-inventories/2017-national-emissions-inventory-nei-technical-support-document-tsd (EPA, 2021).

The full NEI is developed every three years, with 2017 being the most recent year represented wih a full NEI. Large point sources are required to submit to the NEI in interim years, including the year 2018. Point source data representing 2018, including data submitted to EIS by S/L/T agencies, were used for this study. EPA used the SMARTFIRE2 system and the BlueSky Pipeline (https://github.com/pnwairfire/bluesky) emissions modeling system to develop year 2018 fire emissions. SMARTFIRE2 categorizes all fires as either prescribed burning or wildfire categories, and the BlueSky Pipeline system includes fuel loading, consumption and emission factor estimates for both types of fires. Onroad and nonroad mobile source emissions were developed for this project for the year 2018 by running MOVES3 (https://www.epa.gov/moves).

With the exception of onroad, nonroad and fire emissions, Canadian and Mexican emissions were based on those developed for the EQUATES project. The latest year for which inventories were provided was 2016, while the onroad and nonroad emissions adjusted to represent the year 2018.

The emissions modeling process performed using SMOKE, 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 inventories within the emissions modeling platform are separated into sectors for groups of related emissions source categories that are run through all of the SMOKE programs, except the final merge, independently from emissions categories in the other sectors. The final merge program called Mrggrid combines low-level sector-specific gridded, speciated and temporalized emissions to create the final CMAQ-ready emissions inputs. For biogenic and fertilizer emissions, CMAQ allows for these emissions to either be included in the CMAQ-ready emissions inputs, or to be computed within CMAQ itself (the "inline" option). This study uses the inline biogenic emissions option and the CMAQ bidirectional ammonia process for fertilizer emissions.

Table 3-1 presents the sectors in the emissions modeling platform used to develop the year 2018 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 emission summaries for the U.S. sectors are shown in Table 3-2. 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_2018_emissions_totals_by_sector.xlsx".

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

Platform Sector *(Abbrev)*	NEI Category	Description and resolution of the data input to SMOKE
Point source aircraft (*airports*)	Point	2017 NEI point source emissions from airports, including aircraft and airport ground support emissions, adjusted to 2018 using Terminal Area Forecast (TAF) data. Airport-specific factors were used where available, state average factors were used for regional airports, and no change was made to military aircraft from 2017. Annual resolution.
EGUs (*ptegu*)	Point	2018 NEI point source EGUs, with NO_X and SO_2 emissions replaced with hourly Continuous Emissions Monitoring System (CEMS) values, and the remaining pollutants temporally allocated according to CEMS heat input for units that could be matched to the NEI. Emissions for all sources not matched to CEMS data come from 2018 NEI point inventory. Annual resolution for sources not matched to CEMS data, hourly for CEMS sources. EGUs closed in 2018 are not part of the inventory.
Point source oil and gas (*pt_oilgas*)	Point	2018 point sources that include oil and gas production emissions processes for facilities with North American Industry Classification System (NAICS) codes related to Oil and Gas Extraction, Natural Gas Distribution, Drilling Oil and Gas Wells, Support Activities for Oil and Gas Operations, Pipeline Transportation of Crude Oil, and Pipeline Transportation of Natural Gas. Includes U.S. offshore oil production. Production-related sources that did not have 2018 data were pulled forward from the 2017 NEI and adjusted to 2018. Annual resolution.
Remaining non-EGU point (*ptnonipm*)	Point	Includes 2018 reported point sources not matched to the airports, ptegu, or pt_oilgas sectors. Closures were reviewed and implemented based on the most recent submissions to the Emissions Inventory System (EIS). Added a unit from the Kennecott copper mine near Salt Lake City. Includes 2017 NEI rail yard emissions, adjusted to 2018 using same projection factors as the rail sector. Annual resolution.
Point source fire (*ptfire*)	Fires	Point source day-specific wildfires and prescribed fires for 2018 computed using SMARTFIRE2 and BlueSky Pipeline. The ptfire emissions were run as two separate sectors: ptfire-rx (prescribed, including Flint Hills / grasslands) and ptfire-wild.
Point Source agricultural fires (*ptagfire*)	Nonpoint	Agricultural fire sources for year 2018 that were developed by EPA as point and day-specific emissions. Only EPA-developed ag. Fire data are used in this study. Agricultural fires are in the nonpoint data category of the NEI, but in the modeling platform, they are treated as day-specific point sources. Updated HAP-augmentation factors were applied.

Platform Sector *(Abbrev)*	NEI Category	Description and resolution of the data input to SMOKE
Livestock (*livestock*)	Nonpoint	2017 NEI nonpoint livestock emissions adjusted to 2018 using USDA survey data. Livestock includes ammonia and other pollutants (except $PM_{2.5}$). County and annual resolution.
Area fugitive dust (*afdust_adj*)	Nonpoint	PM_{10} and $PM_{2.5}$ fugitive dust sources from the 2017 NEI nonpoint inventory; including building construction, road construction, agricultural dust, and paved and unpaved road dust; adjusted to 2018 based on vehicle miles traveled (VMT). The emissions modeling system applies a transport fraction reduction and a zero-out based on 2018 gridded hourly meteorology (precipitation and snow/ice cover). Emissions are county and annual resolution.
Biogenic (*beis*)	Nonpoint	Year 2018 emissions from biogenic sources. These were left out of the CMAQ-ready merged emissions, in favor of inline biogenic emissions produced during the CMAQ model run itself. Version 5 of the Biogenic Emissions Landuse Database (BELD5) and the Biogenic Emissions Inventory System (BEIS) version 3.7 inputs were used
C1 and C2 commercial marine (*cmv_c1c2*)	Nonpoint	2017 NEI Category 1 (C1) and Category 2 (C2), commercial marine vessel (CMV) emissions based on Automatic Identification System (AIS) data, adjusted to 2018. Point and hourly resolution. Older "Emission Control Area (ECA)" inventory and non-AIS Canada emissions are unchanged from 2017 EQUATES.
C3 commercial marine (*cmv_c3*)	Nonpoint	Within state and federal waters, 2017 NEI Category 3 commercial marine vessel (CMV) emissions based on AIS data, adjusted to 2018. Older "ECA" inventory and non-AIS Canada portion are unchanged from 2017 EQUATES. Point and hourly resolution.
Remaining nonpoint (*nonpt*)	Nonpoint	2017 NEI nonpoint sources not included in other platform sectors. No adjustments were made to represent 2018. County and annual resolution.
Nonpoint source oil and gas (*np_oilgas*)	Nonpoint	Nonpoint 2017 NEI sources from oil and gas-related processes, projected to 2018 using based on U.S. Energy Information Administration (EIA) and Railroad Commission of Texas (TXRRC) historical production data. County and annual resolution.
Fertilizer	Nonpoint	2018 fertilizer ammonia emissions computed inline within CMAQ.
Residential Wood Combustion (*rwc*)	Nonpoint	2017 NEI nonpoint sources with residential wood combustion (RWC) processes were used as is, with no projection to represent 2018. County and annual resolution.
Locomotive (*rail*)	Nonpoint	Line haul rail locomotives emissions for year 2017, projected to 2018 using annual energy outlook (AEO) and additional factors supplied by ERTAC. County and annual resolution.

Platform Sector *(Abbrev)*	NEI Category	Description and resolution of the data input to SMOKE
Volatile chemical products (vcp*)*	Nonpoint	Volatile chemical product (i.e., solvent) emissions for the year 2018 (Seltzer, 2021). Includes household cleaners, personal care products, adhesives, architectural and aerosol coatings, printing inks, and pesticides. Annual and county resolution.
Nonroad (*nonroad*)	Nonroad	2018 nonroad equipment emissions developed with MOVES3, including the updates made to spatial apportionment that were developed with the 2016v1 platform. MOVES3 was used for all states except California, which submitted their own emissions for the 2017 NEI that were adjusted to 2018. County and monthly resolution. California emissions were interpolated to 2018 between California-provided 2017 and 2023 emissions.
Onroad (*onroad*)	Onroad	Onroad mobile source gasoline and diesel vehicles from parking lots and moving vehicles. Includes the following emission processes: exhaust, extended idle, auxiliary power units, evaporative, permeation, refueling, vehicle starts, off network idling, long-haul truck hoteling, and brake and tire wear. Activity data were projected from 2017 to 2018 using factors developed using data from Federal Highway Administration and state departments of transportation. MOVES3 was run for 2018 to generate emission factors.
Onroad California (*onroad_ca_adj*)	Onroad	California-provided 2017 CAP and metal HAP onroad mobile source gasoline and diesel vehicles from parking lots and moving vehicles based on Emission Factor (EMFAC) 2017, gridded and temporalized based on outputs from MOVES3. Volatile organic compound (VOC) HAP emissions derived from California-provided VOC emissions and MOVES-based speciation. 2018 was interpolated between 2017 and 2023 emissions from EMFAC2017.
Onroad Canada (*onroad_can*)	Non-US	Monthly onroad mobile inventory for Canada from EQUATES 2016 projected to 2018 using US onroad trends. Separate trends applied to refueling (gas/diesel) and non-refueling (gas/diesel and LD/HD). Province resolution.
Onroad Mexico (*onroad_mex*)	Non-US	Monthly onroad mobile inventory from MOVES-Mexico (municipio resolution) for 2017, adjusted to 2018 using interpolation between 2017 and 2020.
Other area fugitive dust sources (*othafdust*)	Non-US	Area fugitive dust sources from Canada from EQUATES 2016 with transport fraction and snow/ice adjustments based on 2018 meteorological data. Annual and province resolution.
Other nonpoint and nonroad (*othar*)	Non-US	EQUATES 2016 for Canada and Mexico, except Canada nonroad. Projected Canada nonroad to 2018 based on US MOVES3 2018/2016 ratios. 2016 Mexico (municipio resolution, provided by SEMARNAT) nonpoint and nonroad mobile inventories, annual resolution.

Platform Sector *(Abbrev)*	NEI Category	Description and resolution of the data input to SMOKE
Other point fugitive dust sources (*othptdust*)	Non-US	2017 point source fugitive dust sources from Canada EQUATES 2016/2017 with transport fraction and snow/ice adjustments based on 2018 meteorological data. Annual and province resolution.
Other point sources not from the NEI (*othpt*)	Non-US	Canada and Mexico point source emissions from EQUATES 2016. Canada point sources were provided by ECCCC and Mexico point source emissions for 2016 were provided by SEMARNAT. Annual and monthly resolution.
Point fires in Mexico and Canada (*ptfire_othna*)	Non-US	Point source day-specific wildfires and agricultural fires outside of the U.S. for 2018 from v1.5 of the Fire INventory (FINN) from National Center for Atmospheric Research (NCAR, 2017 and Wiedinmyer, C., 2011) for Canada, Mexico, Caribbean, Central American, and other international fires.

Table 3-2. 2018 Continental United States Emissions by Sector (tons/yr in 48 states + D.C.)

Sector	CO	NH₃	NOₓ	PM₁₀	PM₂.₅	SO₂	VOC
afdust_adj				5,691,832	789,322		
airports	489,039	0	131,779	9,813	8,576	16,492	54,939
cmv_c1c2	24,431	86	168,566	4,622	4,480	655	6,674
cmv_c3	15,068	42	114,722	2,380	2,189	4,891	9,311
livestock		2,571,572					225,550
nonpt	1,927,267	102,898	739,250	572,589	475,154	166,399	818,185
nonroad	10,473,047	1,925	988,078	96,182	90,714	1,372	1,016,057
np_oilgas	668,211	15	664,978	11,570	11,397	43,657	2,783,694
onroad	17,043,371	103,249	2,827,451	207,714	88,309	22,628	1,172,608
ptegu	575,731	21,523	1,143,934	159,382	126,097	1,320,882	32,793
ptagfire	421,836	93,685	17,935	59,968	38,050	7,451	63,726
ptfire-rx	10,873,070	177,629	182,473	1,168,800	1,001,912	91,868	2,617,765
ptfire-wild	10,275,916	168,798	147,585	1,051,942	891,476	79,478	2,426,465
ptnonipm	1,387,105	61,531	905,359	387,125	241,089	569,451	609,870
pt_oilgas	178,585	485	366,485	13,077	12,218	39,151	138,835
rail	117,171	365	570,969	15,494	15,005	727	24,947
rwc	2,160,529	16,413	34,093	300,139	299,278	7,988	323,969
vcp							2,886,974
Continental U.S.	**56,630,375**	**3,320,086**	**9,003,657**	**9,752,629**	**4,095,265**	**2,373,089**	**15,212,360**
beis (biogenics)	3,858,461		959,081				25,777,565
fertilizer (bidi)		1,259,282					

Table 3-3. Non-US Emissions by Sector within the 12US1 Modeling Domain (tons/yr for Canada, Mexico, Offshore)

Sector	CO	NH₃	NOₓ	PM₁₀	PM₂.₅	SO₂	VOC
Canada othafdust				580,703	90,421		
Canada othptdust				132,266	46,401		
Canada othar	2,182,369	3,815	306,078	223,090	174,668	16,318	725,957
Canada onroad_can	1,661,932	7,156	331,485	23,592	11,282	1,531	134,046
Canada othpt	1,115,786	348,022	653,888	90,209	43,221	993,759	762,206
Canada ptfire_othna	4,679,983	93,406	195,209	671,858	565,668	38,759	1,343,696
Canada CMV	11,104	37	96,622	1,716	1,594	2,941	5,409
Canada subtotal	**9,651,174**	**452,436**	**1,583,282**	**1,723,433**	**933,256**	**1,053,308**	**2,971,314**

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Sector	CO	NH₃	NOₓ	PM₁₀	PM₂.₅	SO₂	VOC
Mexico othar	115,420	111,699	60,057	104,896	34,686	1,729	361,621
Mexico onroad_mex	1,821,182	2,918	447,430	15,744	11,158	6,638	159,185
Mexico othpt	108,712	1,093	190,460	53,893	37,389	354,827	35,671
Mexico ptfire_othna	438,065	8,465	17,524	57,762	49,343	3,612	126,265
Mexico subtotal	**2,483,380**	**124,175**	**715,472**	**232,294**	**132,576**	**366,807**	**682,743**
Offshore pt_oilgas	51,866	8	49,959	636	635	462	38,803
Offshore CMV to EEZ	34,428	133	292,670	7,437	6,886	29,127	16,779
Non-ECA CMV	24,283	457	267,502	25,810	23,752	189,097	11,528
2018 Non-US Total	**12,210,703**	**577,077**	**2,616,214**	**1,982,174**	**1,090,219**	**1,609,674**	**3,704,388**

3.2.1 Point Sources (ptegu, pt_oilgas, ptnonipm, and airports)

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 CMV emissions (cmv_c1c2 and cmv_c3 sectors) are processed by SMOKE as point source inventories and are discussed later in this section. A complete NEI is developed every three years, with 2017 being the most recently completed NEI. A comprehensive description about the development of the 2017 NEI is available in the 2017 NEI TSD (EPA, 2021). Point inventories are also available in EIS for intermediate years such as 2018. In the intermediate point inventories, states are required to update larger sources with emissions for the interim year, while sources not updated by states are either carried forward from the most recent NEI or marked as closed and removed.

In preparation for modeling, the complete set of point sources in the NEI was exported from EIS for the year 2018 into the Flat File 2010 (FF10) format that is compatible with SMOKE (see https://www.cmascenter.org/smoke/documentation/4.8.1/html/ch08s02s08.html) and was then split into several sectors for modeling. After 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 point sources. The point sectors are: EGUs (ptegu), point source oil and gas extraction-related sources (pt_oilgas), airport emissions (airports), 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) and airport emissions (airports) were processed separately for summary tracking purposes and distinct projection techniques from the remaining non-EGU emissions (ptnonipm).

In some cases, data about facility or unit closures are entered into EIS after the inventory modeling inventory flat were reviewed and implemented based on the most recent submissions to EIS. Prior to processing through SMOKE, submitted closures were reviewed and if closed sources were found in the inventory, those were removed.

For the 2018 platform, an analysis of point source stack parameters (e.g., stack height, diameter, temperature, and velocity) was performed after some specific examples of unrealistic stack parameters as default values were noticed. The defaulted values were noticed in data submissions for the states of Illinois, Louisiana, Michigan, Pennsylvania, Texas, and Wisconsin. Where these defaults were detected and deemed to be unreasonable for the specific process, the affected stack parameters were replaced by values from the currently available PSTK file that is input to SMOKE. PSTK contains default stack parameters by source classification code (SCC). These updates impacted the ptnonipm and pt_oilgas inventories.

The ptnonipm, pt_oilgas, and airports sector emissions were provided to SMOKE as annual emissions. For sources in the ptegu sector that could be matched to 2018 CEMS data, hourly CEMS NO_X and SO_2 emissions for 2018 from EPA's Acid Rain Program were used rather than annual inventory emissions. For all other pollutants (e.g., VOC, $PM_{2.5}$, HCl), annual emissions were used as-is from the annual inventory but were allocated to hourly values using heat input from the CEMS data. For the unmatched units in the ptegu sector, annual emissions were allocated to daily values using 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 ptnonipm sector includes sources that are not modeled by EPA's Integrated Planning Model (IPM) which is used to estimate EGU emissions in future years. The full description of how the NEI emissions were developed is provided in the NEI documentation, but a brief summary of their development follows:

a. CAP and HAP data were provided by States, locals and tribes under the Air Emissions Reporting Rule (AERR) [the reporting size threshold is larger for inventory years between the triennial inventory years of 2011, 2014, 2017, …].

b. EPA corrected known issues and filled PM data gaps.

c. EPA added HAP data from the Toxic Release Inventory (TRI) where corresponding data was not already provided by states/locals.

d. EPA stored and applied matches of the point source units to units with CEMS data and also for all EGU units modeled by IPM.

e. Data for airports and rail yards were incorporated.

f. Off-shore platform data were added from the Bureau of Ocean Energy Management (BOEM).

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

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

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

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 2018 point source inventory that could be matched to units found in the National Electric Energy Database System (NEEDS) v6 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.

The 2018 ptegu emissions inventory is a subset of the point source flat file for 2018 exported from the Emissions Inventory System (EIS). In the point source flat file, emission records for sources that have been matched to the NEEDS database have a value filled into the IPM_YN column based on the matches stored within EIS. Thus, unit-level emissions were split into a separate EGU flat file for units that have a populated (non-null) ipm_yn field. A populated ipm_yn field indicates that a match was found for the EIS unit in the NEEDS v6 database. Updates were made to the flat file output from EIS as described in the list below:

- ORIS facility and unit identifiers were updated based on additional matches in a cross-platform spreadsheet, based on state comments, and using the EIS alternate identifiers table as described later in this section.

Some units in the ptegu sector are matched to Continuous Emissions Monitoring System (CEMS) data via Office of Regulatory Information System (ORIS) facility codes and boiler IDs. For the matched units, the annual emissions of NO_X and SO_2 in the flat file are replaced with the hourly CEMS emissions in base year modeling. For other pollutants at matched units, the hourly CEMS heat input data are used to allocate the NEI annual emissions to hourly values. All stack parameters, stack locations, and Source Classification Codes (SCC) for these sources come from the flat file. If CEMS data exists for a unit, but the unit is not matched to the NEI, the CEMS data for that unit are not used in the modeling platform. However, if the source exists in the NEI and is not matched to a CEMS unit, the emissions from that source are still modeled using the annual emission value in the NEI temporally allocated to hourly values.

EIS stores many matches from NEI units to the ORIS facility codes and boiler IDs used to reference the CEMS data. In the flat file, emission records for point sources matched to CEMS data have values filled into the ORIS_FACILITY_CODE and ORIS_BOILER_ID columns. The CEMS data are available at http://ampd.epa.gov/ampd near the bottom of the "Prepackaged Data" tab. Many smaller emitters in the CEMS program cannot be matched to the NEI due to inconsistencies in the way a unit is defined between the NEI and CEMS datasets, or due to uncertainties in source identification such as inconsistent plant names in the two data systems. In addition, the NEEDS database of units modeled by IPM includes many smaller emitting EGUs that do not have CEMS. Therefore, there will be more units in the ptegu sector than have CEMS data.

For the 2016 platform, matches from the NEI to ORIS codes and the NEEDS database were improved. The matching improvements were carried forward to the 2017 and 2018 platforms where applicable. In some cases, NEI units in EIS match to many CAMD units. In these cases, a new entry was made in the flat file with a "_M_" in the ipm_yn field of the flat file to indicate that there are "multiple" ORIS IDs that match that unit. This helps facilitate appropriate temporal allocation of the emissions by SMOKE. Temporal allocation for EGUs is discussed in more detail in the Ancillary Data section below. A cross reference between NEEDS, NEI, and ERTAC is available here: https://gaftp.epa.gov/Air/emismod/2016/v1/reports/EGU/egu_2016_2023_2030_NEEDS_NEI_ERTAC_xref_13jun2019.xlsx.

The EGU flat file was split into two flat files: those that have unit-level matches to CEMS data using the oris_facility_code and oris_boiler_id fields and those that do not so that different temporal profiles could be applied. In addition, the hourly CEMS data were processed through v2.1 of the CEMCorrect tool to mitigate the impact of unmeasured values in the data.

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 2017 oil and gas emissions can be found in Section 4.17 of the 2017 NEI TSD. The pt_oilgas sector includes emissions from offshore oil platforms. Where available, the point source emissions submitted as part of the 2018 NEI process were used. For sources that otherwise would be pulled forward with 2017 emissions values because 2018-specific emissions were not available, projection factors by NAICS and state, were applied to those 2017 sources to adjust the emissions to make them more representative of 2018. Texas has district-specific factors instead of state-specific, which were applied. State (plus TX Railroad Commission district) factors were applied to production-related NAICS. Transportation NAICS were projected using nationally derived production-related factors for oil and gas. All other NAICS were held constant from 2017 NEI. All Tribal data and offshore emissions are held constant from 2017 NEI.

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

NAICS	NAICS description
2111	Oil and Gas Extraction
211111	Crude Petroleum and Natural Gas Extraction
211112	Natural Gas Liquid Extraction
21112	Crude Petroleum Extraction
211120	Crude Petroleum Extraction
21113	Natural Gas Extraction
211130	Natural Gas Extraction
213111	Drilling Oil and Gas Wells
213112	Support Activities for Oil and Gas Operations
2212	Natural Gas Distribution
22121	Natural Gas Distribution

NAICS	NAICS description
221210	Natural Gas Distribution
237120	Oil and Gas Pipeline and Related Structures Construction
4861	Pipeline Transportation of Crude Oil
48611	Pipeline Transportation of Crude Oil
486110	Pipeline Transportation of Crude Oil
4862	Pipeline Transportation of Natural Gas
48621	Pipeline Transportation of Natural Gas
486210	Pipeline Transportation of Natural Gas

3.2.1.3 *Airports Sector (airports)*

Emissions at airports were separated from other sources in the point inventory based on sources that have the facility source type of 100 (airports). The airports sector includes all aircraft types used for public, private, and military purposes and aircraft ground support equipment. The Federal Aviation Administration's (FAA) Aviation Environmental Design Tool (AEDT) is used to estimate emissions for this sector. For 2017, Texas and California submitted aircraft emissions. Additional information about aircraft emission estimates can be found in section 3.2.2 of the 2017 NEI TSD. Terminal Area Forecast (TAF) data were used to project 2017 NEI emissions to 2018. EPA used airport-specific factors where available. Regional airports were projected using state average factors. Military airports were unchanged from 2017. An update for the 2018 platform was that airport emissions were spread out into multiple 12km grid cells when the airport runways were determined to overlap multiple grid cells. Otherwise, airport emissions for a specific airport are confined to one air quality model grid cell.

3.2.1.4 *Non-IPM Sector (ptnonipm)*

With some exceptions, the non-IPM (ptnonipm) sector contains the point sources that are not in the ptegu, pt_oilgas, or airports sectors. For the most part, the ptnonipm sector reflects the non-EGU sources. However, it is likely that some low-emitting EGUs not matched to the NEEDS database or to CEMS data may be found in the ptnonipm sector.

For 2018, the Kennecott copper mine near Salt Lake City, Utah was determined to be missing from the inventory. It was added prior to processing through SMOKE.

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.

The ptnonipm sources (i.e., not EGUs and non -oil and gas sources) were used as-is from the 2018 NEI point inventory with the exception of the volatile chemical products (vcp) sector. The vcp sector is a diverse collection of solvent emission sources whose emissions are driven by evaporation. Included in this sector are everyday items, such as cleaners, personal care products, adhesives, architectural and

aerosol coatings, printing inks, and pesticides. Any sources that overlap the vcp sector were removed from the point source inventory. The vcp sector is described in more detail in Section 3.2.3.6.

Emissions from railyards are included in the ptnonipm sector. Railyards were projected to 2018 from the 2017 NEI railyard inventory, using factors derived from the Annual Energy Outlook 2018 (https://www.eia.gov/outlooks/archive/aeo18/).

3.2.2 Day-Specific Point Source Fires (ptfire)

Wildfire and prescribed burning emissions are contained in the ptfire-rx and ptfire-wild sectors. Both ptfire sectors have 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.

Figure 3-1 shows the processing stream for wildfire and prescribed burn sources. The emissions estimate methodology consists of two tools or systems. The first system is called Satellite Mapping Automated Reanalysis Tool for Fire Incident Reconciliation version 2 (SMARTFIRE2). SMARTFIRE2 is an algorithm and database system that operate within a geographic information system (GIS) framework. SMARTFIRE2 combines multiple sources of fire information and reconciles them into a unified GIS database. It reconciles fire data from space-borne sensors and ground-based reports, thus drawing on the strengths of both data types while avoiding double-counting. At its core, SMARTFIRE2 is an association engine that links reports covering the same fire in any number of multiple databases. In this process, all input information is preserved, and no attempt is made to reconcile conflicting or potentially contradictory information (for example, the existence of a fire in one database but not another). In this study, the national and S/L/T fire information is input into SMARTFIRE2 and then all information is merged and associated together based on user-defined weights for each fire information dataset. The output from SMARTFIRE2 is daily acres burned and latitude-longitude coordinates for each fire.
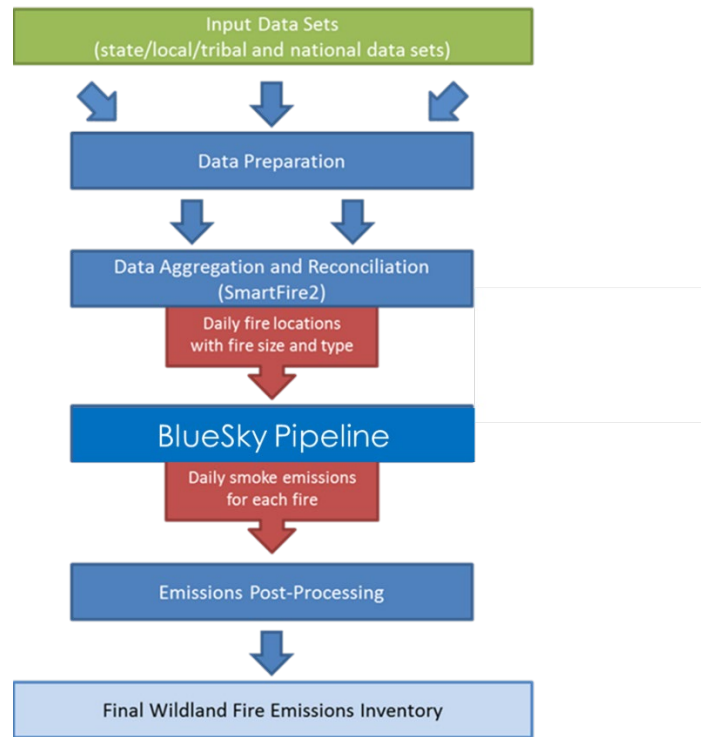
Figure 3-1. Processing flow for fire emission estimates

Inputs to SMARTFIRE2 for 2018 included:

- The National Oceanic and Atmospheric Administration's (NOAA's) Hazard Mapping System (HMS) fire location information
- GeoMAC (Geospatial Multi-Agency Coordination), an online wildfire mapping application designed for fire managers to access maps of current fire locations and perimeters in the United States
- The Incident Status Summary, also known as the "ICS-209", used for reporting specific information on fire incidents of significance
- Incident reports including dates of fire activity, acres burned, and fire locations from the National Association of State Foresters (NASF)
- Hazardous fuel treatment reduction polygons for prescribed burns from the Forest Service Activity Tracking System (FACTS)
- Fire activity on federal lands from the United States Fish and Wildlife Service (USFWS)
- Wildfire and prescribed date, location, and locations from S/L/T activity submitters
  - o Included data from Kansas, Georgia, and Florida

The second system used to estimate emissions is the BlueSky Pipeline modeling system (version 4.2.14). The BlueSky Pipeline system supports the calculation of fuel loading and consumption, and emissions using various models depending on the available inputs as well as the desired results. The contiguous United States and Alaska, where Fuel Characteristic Classification System (FCCS) fuel loading data are available, were processed using the modeling chain described in Figure 3-2. The Fire Emissions Production Simulator (FEPS) in the BlueSky Pipeline generates all the CAP emission factors for wildland

fires used in this 2018 study. HAP emission factors were obtained from Urbanski's (2014) work and applied by region and by fire type.
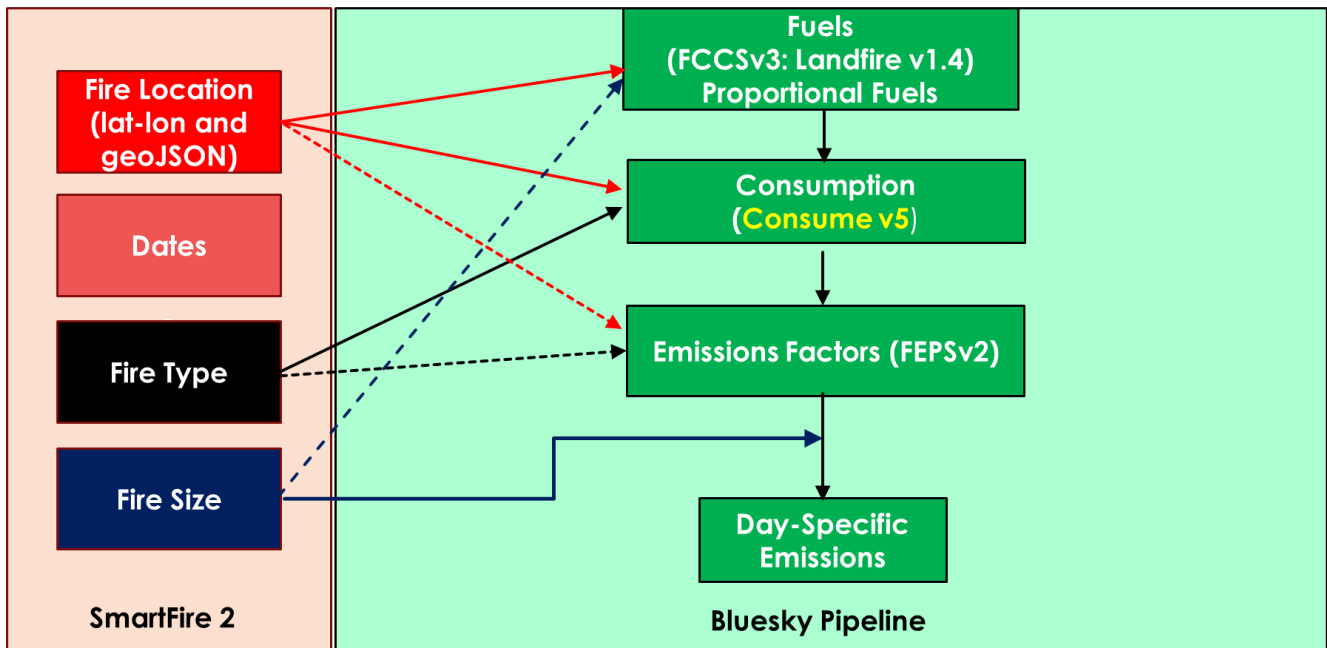

Figure 3-2. BlueSky Pipeline modeling system

The FCCSv3 cross-reference was implemented along with the LANDFIREv1.4 (at 200-meter resolution) to provide better fuel bed information for the BlueSky Pipeline (BSP). The LANDFIREv1.4 was aggregated from the native resolution and projection to 200 meter using a nearest-neighbor methodology. Aggregation and reprojection was required for the proper function on BSP.

The final products from this process are annual and daily FF10-formatted emissions inventories. These SMOKE-ready inventory files contain both CAPs and HAPs. The BAFM HAP emissions from the inventory were used directly in modeling and were not overwritten with VOC speciation profiles (i.e., an "integrate HAP" use case).

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

Several modeling platform sectors were created from the 2017 NEI nonpoint inventory. This section describes the *stationary* nonpoint sources. Locomotives, C1 and C2 CMV, and C3 CMV are also included the NEI nonpoint data category but are mobile sources and are described in a later section. The 2017 NEI 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 sources in the nonpoint NEI data category were 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 based on the meteorological data for the year being modeled. 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 are accounted for in the subsequent meteorological adjustment.

Paved road dust emissions were projected from 2017 (January 2021 version) to 2018 based on county-level VMT trends. All other afdust SCCs were held constant from the 2017 NEI. For the data compiled into the NEI, meteorological adjustments are applied to paved and unpaved road SCCs but not transport adjustments. This is because the modeling platform applies meteorological adjustments and transport adjustments based on unadjusted NEI values. For the 2018 platform, the meteorological adjustments that were applied (to paved and unpaved road SCCs) were backed out in order reapply them in SMOKE. The FF10 that is run through SMOKE consists of 100% unadjusted emissions, and after SMOKE all afdust sources have both transport and meteorological adjustments applied according to year 2018 meteorology.

For categories other than paved and unpaved roads, 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 for sources other than paved and unpaved roads, 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 Livestock Sector (livestock)*

 The livestock emissions in this sector are based only on the SCCs starting with 2805. The livestock SCCs are related to beef and dairy cattle, poultry production and waste, swine production, waste from horses and ponies, and production and waste for sheep, lambs, and goats. The sector does not include quite 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 addition to NH_3, the sector includes livestock emissions from all pollutants other than $PM_{2.5}$. $PM_{2.5}$ from livestock are in the afdust sector.

Agricultural livestock emissions in the 2018 platform were projected from the 2017 NEI (January 2021 version), which is a mix of state-submitted data and EPA estimates. USDA Survey data for 2017 and 2018 was used to create projection factors (https://quickstats.nass.usda.gov/) . Livestock emissions utilized improved animal population data. VOC livestock emissions, new for this sector, were estimated by multiplying a national VOC/NH_3 emissions ratio by the county NH_3 emissions. The 2017 NEI approach for livestock utilizes daily emission factors by animal and county from a model developed by Carnegie Mellon University (CMU) (Pinder, 2004, McQuilling, 2015) and 2017 U.S. Department of Agriculture (USDA) National Agricultural Statistics Service (NASS) survey. Details on the approach are provided in Section 4.5 of the 2017 NEI TSD.

3.2.3.2   *Agricultural Fertilizer Sector (fertilizer)*

As described in the 2017 NEI TSD, fertilizer emissions are based on the FEST-C model (https://www.cmascenter.org/fest-c/). The bidirectional version of CMAQ (v5.3) and the Fertilizer Emissions Scenario Tool for CMAQ FEST-C (v1.3) were used within CMAQ to estimate ammonia (NH_3) emissions from agricultural soils. The approach to estimate year-specific fertilizer emissions consists of these steps:

- Run FEST-C and CMAQ model with bidirectional ("bidi") NH_3 exchange to produce nitrate (NO_3), Ammonium (NH4+, including Urea), and organic (manure) nitrogen (N) fertilizer usage estimates, and gaseous ammonia NH_3 emission estimates respectively.

- Calculate county-level emission factors as the ratio of bidirectional CMAQ NH_3 fertilizer emissions to FEST-C total N fertilizer application.

- Assign the NH_3 emissions to one SCC: "…Miscellaneous Fertilizers" (2801700099).

For livestock and fertilizer, meteorological-based temporalization (described in Section 3.3.5.3) is used for month-to-day and day-to-hour temporalization. Monthly profiles for livestock are based on the daily data underlying the EPA estimates from 2014NEIv2. The fertilizer inventory includes monthly emissions from FEST-C and uses the same meteorological-based month-to-hour profiles as livestock in the same way as was done for other recent platforms.

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 for the year 2018 in a similar way to the emissions in ptfire. The state of Florida provided their own emissions (separate from the other states) for this study.

Daily year-specific agricultural burning emissions are derived from HMS fire activity data, which contains the date and location of remote-sensed anomalies. The activity is filtered using the 2018 USDA cropland data layer (CDL). Satellite fire detects over agricultural lands are assumed to be agricultural burns and assigned a crop type. Detects that are not over agricultural lands are output to a separate file for use in the ptfire sector. Each detect is assigned an average size of between 40 and 80 acres based on crop

type. Grassland/pasture fires were moved to the ptfire sectors for this 2018 modeling platform. Depending on their origin, grassland fires are in both ptfire-rx and ptfire-wild sectors because both fire types do involve grassy fuels.

Another feature of the database is that the satellite detections for 2018 were filtered out to exclude areas covered by snow during the winter months. To do this, the daily snow cover fraction per grid cell was extracted from a 2018 meteorological simulation (WRF). The location of fire detections was then compared with this daily snow cover file. For any day in which a grid cell has snow cover, that fire detection was excluded.   Due to the inconsistent reporting of fire detections from the Visible Infrared Imaging Radiometer Suite (VIIRS) platform, any fire detections in the HMS dataset that were flagged as VIIRS or SUOMI were excluded. In addition, certain crop types (corn and soybeans) have been excluded from these specific midwestern states: Iowa, Kansas, Indiana, Illinois, Michigan, Missouri, Minnesota, Wisconsin, and Ohio. Emissions factors were applied to each daily fire to calculate criteria and hazardous pollutant values. These factors vary by crop type.

Heat flux for plume rise was calculated using the size and assumed fuel loading of each daily agricultural fire. This information is needed for a plume rise calculation within a chemical transport modeling system.

The daily agricultural and open burning emissions were converted from a tabular format into the SMOKE-ready daily point flat file format. The daily emissions were also aggregated into annual values by location and converted into the annual point flat file format.

For this modeling platform, a SMOKE update allows the use of HAP integration for speciation for PTDAY inventories. The 2018 agricultural fire inventories include emissions for HAPs, so HAP integration was used for this study.

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 2017 oil and gas activity data with the Oil and Gas Tool, and many S/L/T agencies also submitted nonpoint oil and gas data for the 2017 NEI. 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.

EPA has updated the Nonpoint Oil and Gas Emission Estimation Tool (i.e., the "tool") to estimate emissions. Year 2017 oil and gas activity data was supplied to EPA by state air agencies and where state data is not supplied to EPA, EPA populated the 2017 inventory with the best available data. The tool is an Access database that utilizes county-level activity data (e.g., oil production and well counts), operational characteristics (types and sizes of equipment), and emission factors to estimate emissions.   The tool creates a CSV-formatted emissions dataset covering all national nonpoint oil and gas emissions. This dataset is then converted to FF10 format for use in SMOKE modeling. More details on the inputs for and running of the tool are provided in the 2017 NEI TSD.

The 2017 NEI inventory was projected to 2018 using factors by SCC and state. SCCs are grouped into exploration (all fuels) and production (oil/gas/both). Factors were state-specific except Texas, where they were district-specific. The exploration data used to generate the exploration-factors was from the Baker-

Hughes rig count database. The production data used to generate the production-factors was from EIA and TXRRC website historical databases.

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 chimeneas. 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.

The 2018 platform RWC is unchanged from the data in the 2017 NEI. Some improvements to RWC emissions estimates were made for the 2017 NEI and were included in this study. The EPA, along with the Commission on Environmental Cooperation (CEC), the Northeast States for Coordinated Air Use Management (NESCAUM), and Abt Associates, conducted a national survey of wood-burning activity in 2018. The results of this survey were used to estimate county-level burning activity data. The activity data for RWC processes is the amount of wood burned in each county, which is based on data from the CEC survey on the fraction of homes in each county that use each wood-burning appliance and the average amount of wood burned in each appliance. These assumptions are used with the number of occupied homes in each county to estimate the total amount of wood burned in each county, in cords for cordwood appliances and tons for pellet appliances. Cords of wood are converted to tons using county-level density factors from the U.S. Forest Service. RWC missions were calculated by multiplying the tons of wood burned by emissions factors. For more information on the development of the residential wood combustion emissions, see Section 4.15 of the 2017 NEI TSD.

3.2.3.6　　　　*Volatile Chemical Products (vcp)*

The solvents sector is a diverse collection of emission sources whose emissions are driven by evaporation. Included in this sector are everyday items, such as cleaners, personal care products, adhesives, architectural and aerosol coatings, printing inks, and pesticides. These sources exclusively emit organic gases and feature origins spanning residential, commercial, institutional, and industrial settings. The organic gases that evaporate from these sources often fulfill other functions than acting as a traditional solvent (e.g., propellants, fragrances, emollients); as such, this sector is frequently described as the volatile chemical product (VCP) sector.

Here, emissions from the solvent sector are derived using the VCPy framework (Seltzer et al., 2021). The VCPy framework is based on the principle that the magnitude and speciation of organic emissions from this sector are directly related to (1) the mass of chemical products used, (2) the composition of these products, (3) the physiochemical properties of their constituents that govern volatilization, and (4) the timescale available for these constituents to evaporate. National product usage is preferentially estimated using economic statistics from the U.S. Census Bureau's Annual Survey of Manufacturers (U.S. Census Bureau, 2021), commodity prices from the U.S. Department of Transportation's 2012 Commodity Flow Survey (U.S. Department of Transportation, 2015) and the U.S. Census Bureau's Paint and Allied Products Survey (U.S. Census Bureau, 2011), and producer price indices, which scale commodity prices to target years, are retrieved from the Federal Reserve Bank of St. Louis (U.S. Bureau of Labor Statistics,

2020). In circumstances where the aforementioned datasets are unavailable, default usage estimates are derived using functional solvent usage reported by a business research company (The Freedonia Group, 2016) or in sales reported in a California Air Resources Board (CARB) California-specific survey (CARB, 2019). The composition of products is estimated by generating composites from various CARB surveys (CARB, 2007; CARB, 2012; CARB 2014; CARB, 2018; CARB, 2019) and profiles reported in the U.S. EPA's SPECIATE database (EPA, 2019). For oil and gas solvent usage, the composition is assumed to be dominated by methanol and other hydrocarbon blends. The physiochemical properties of all organic components are generated from the quantitative structure-activity relationship model OPERA (Mansouri et al., 2018) and the characteristic evaporation timescale of each component is estimated using previously published methods (Khare and Gentner, 2018; Weschler and Nazaroff, 2008).

National-level emissions are then allocated to the county-level using several proxies. Most emissions are allocated using population as a spatial surrogate. This includes all cleaners, personal care products, adhesives, architectural coatings, and aerosol coatings. Industrial coatings, allied paint products, printing inks, and dry cleaning emissions are allocated using county-level employment statistics from the U.S. Census Bureau's County Business Patterns (U.S. Census Bureau, 2018) and follow the same mapping scheme used in the U.S. EPA's 2017 National Emissions Inventory (U.S. EPA, 2020). Agricultural pesticides are allocated using county-level agricultural pesticide use, as taken from the 2017 NEI and oil and gas emissions are allocated using oil and gas well counts (U.S. EIA, 2019).

3.2.3.6   *Other Nonpoint Sources (nonpt)*

The 2018 platform nonpt sector inventory is mostly unchanged from the January 2021 version of the 2017 NEI. 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 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;

- 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; and

- 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.

Volatile chemical product (aka solvent) SCCs were removed from the nonpt sector and placed into the vcp sector. The EPA incorporated new methods to estimate emissions of VOC and associated HAPs from the vcp sector, for this 2018 modeling platform (See section 3.2.3.6 for details). The new methods result in improved emissions estimates for the nonpoint (county-wide) solvent emissions. The new emissions method results in improved VOC and HAP estimates for nonpoint categories of coatings, pesticides, adhesives and sealants, oil & gas exploration solvent use, dry cleaning, printing inks, cleaning products, personal care products, and other miscellaneous solvent uses.

3.2.4 Biogenic Sources (beis)

Biogenic emissions were computed based on the 18j version of the 2018 meteorological data used for the air quality modeling and were developed using the Biogenic Emission Inventory System version 3.7 (BEIS3.7) within CMAQ. The BEIS3.7 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 3.7 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 3.7

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

Variable	Description
RADYNI	inverse of aerodynamic resistance
TEMP2	temperature at 2 m

BEIS3.7 was used in conjunction with Version 5 of the Biogenic Emissions Landuse Database (BELD5). The BELD5 is based on an updated version of the USDA-USFS Forest Inventory and Analysis (FIA) vegetation speciation-based data from 2001 to 2017 from the FIA version 8.0. This same configuration of BEIS3.7 and BELD5 was used to develop the biogenic emissions in the 2017 NEI. Canopy coverage is based on the Global Moderate Resolution Imaging Spectroradiometer (MODIS) 20 category data with enhanced lakes and Fraction of Photosynthetically Active Radiation (FPAR) for vegetation coverage from National Center for Atmospheric Research (NCAR). 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 MODIS canopy coverage. For land areas outside the conterminous United States, 500-meter grid spacing land cover data from the MODIS is used. BELD5 also incorporates the following:

- Canadian BELD land use, Updates to Version 4 of the Biogenic Emissions Landuse Database (BELD4) for Canada and Impacts on Biogenic VOC Emissions (https://www.epa.gov/sites/production/files/2019-08/documents/800am_zhang_2_0.pdf)
- 2017 30 meter USDA Cropland Data Layer (CDL) data (http://www.nass.usda.gov/research/Cropland/Release/).

Biogenic emissions computed with BEIS to review and prepare summaries, but they were left out of the CMAQ-ready merged emissions. Instead, the biogenic emissions are produced inline during the CMAQ model run which uses the same algorithm described above, but with finer time steps within the air quality model.

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 ocean-going Category 3 vessels are in the cmv_c3 sector. Both CMV sectors 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 CMV to be modeled with plume rise.

3.2.5.1 Onroad (onroad)

Onroad mobile sources include emissions from motorized vehicles that 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 the 2018 modeling platform, VMT were projected from 2017 to 2018 based mostly on Federal Highways administration (FHWA) annual VMT changes at the county level. In a few cases, state Department of Transportation (DOT) data were used instead of FHWA data. Other activity data (i.e., starts, on-network idling, VPOP, and hoteling) are projected by applying a ratio of 2017-based VMT/activity ratios to the 2018 VMT. For more details on the approach and for a summary of the MOVES inputs submitted by states, see section 6.5.1 of the 2017 NEI TSD. In addition, a number of states submitted 2017-specific activity data for incorporation into this platform. Finally, a new MOVES run for 2018 was done using MOVES3.

MOVES3 includes the following updates from MOVES2014b:
- Updated emission rates:
    - Updated heavy-duty (HD) diesel running emission rates based on manufacturer in-use testing data from hundreds of HD trucks
    - Updated HD gasoline and compressed natural gas (CNG) trucks
    - Updated light-duty (LD) emission rates for hydrocarbons (HC), CO, NOx, and PM
- Includes updated fuel information
- Incorporates HD Phase 2 Greenhouse Gas (GHG) rule, allowing for finer distinctions among HD vehicles
- Accounts for glider vehicles that incorporate older engines into new vehicle chassis
- Accounts for off-network idling – emissions beyond the idling that is already considered in the MOVES drive cycle
- Includes revisions to inputs for hoteling
- Adds starts as a separate type of rate and activity data

Except for California, onroad emissions are generated using the SMOKE-MOVES interface that leverages MOVES generated emission factors (https://www.epa.gov/moves), 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, VMT, VPOP, starts, 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. Meteorological data were specific to the year 2018.

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 2018-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, and inspection and maintenance (I&M) 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 329 representative counties in the continental U.S. The representative counties that were used for the 2018 platform are very close to what was used in EPA's Air Quality Time Series (EQUATES) project for 2016/2017. The EPA added some additional representative counties to the set used for EQUATES to account for altitude and variations in I&M programs and fuels.

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 then 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 (RPS) uses STARTS activity data to compute off-network emissions from vehicles starts;

- 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 (RPHO) uses off network idling hours activity data to compute off-network idling emissions for all types of vehicles; 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 2018 platform are based on the 2017 NEI, described in more detail in Section 6 of the 2017 NEI TSD. These inputs include:

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

Fuel months and other inputs were consistent with those in the 2017 NEI, although age distributions were adjusted to represent the year 2018. A list of states that submitted activity data along with a description of the development of the EPA default activity data sets for VMT, VPOP, and hoteling hours are available in detail in the 2017 NEI TSD and supporting documents. Hoteling hours activity are used to calculate emissions from extended idling and auxiliary power units (APUs) by combination long-haul trucks.

Hoteling hours were capped by county at a theoretical maximum and any excess hours of the maximum were reduced. For calculating reductions, a dataset of truck stop parking space availability was used, which includes a total number of parking spaces per county. This same dataset is used to develop the spatial surrogate for allocating county-total hoteling emissions to model grid cells. The parking space dataset includes several recent updates based on new truck stops opening and other new information. There are 8,760 hours in the year 2018; therefore, the maximum number of possible hoteling hours in a particular county is equal to 8,760 * the number of parking spaces in that county. Hoteling hours were capped at that theoretical maximum value for 2018 in all counties, with some exceptions.

Because the truck stop parking space dataset may be incomplete in some areas, and trucks may sometimes idle in areas other than designated spaces, it was assumed that every county has at least 12 parking spaces, even if fewer parking spaces are found in the parking space dataset. Therefore, hoteling hours are never reduced below 105,408 hours for the year in any county. If the unreduced hoteling hours were already below that maximum, the hours were left unchanged; in other words, hoteling activity are never increased as a result of this analysis. Four states requested that no reductions be applied to the hoteling activity based on parking space availability: CO, ME, NJ, and NY. For these states, reductions based on parking space availability were not applied.

The final step related to hoteling activity is to split county totals into separate values for extended idling (SCC 2202620153) and Auxiliary Power Units (APUs) (SCC 2202620191). New Jersey's submittal of hoteling activity specified a 30% APU split, and this was used throughout NJ. For the rest of the country, a 12.4% APU split was used, meaning that during 12.4% of the hoteling hours auxiliary power units are assumed to be running.

The last pieces of activity data needed for SMOKE-MOVES are related to the average speed of vehicles, which affects the selection of MOVES emission factors for on-network emissions. One such dataset is the SPEED inventory read by the SMOKE program Smkinven, which includes a single overall average speed

for each county, SCC, and month. The second dataset is the SPDIST dataset read by the SMOKE program Movesmrg, which specifies the amount of time spent in each MOVES speed bin for each county, vehicle (aka source) type, road type, weekday/weekend, and hour of day. SMOKE still requires the SPEED dataset exist even when hourly speed data is available, even though only the hourly speed data affects the selection of emission factors. The SPEED and SPDIST datasets are from the 2017 NEI with some of the data carried over from the Coordinating Research Council A-100 study (CRC, 2017).

MOVES3 was run in emission factor mode to create emission factor tables using CB6 speciation for the year 2018, for all representative counties and fuel months. The county databases used to run MOVES to develop the emission factor tables included the state-specific control measures such as the California LEV program, and fuels represented the year 2018. The range of temperatures run along with the average humidities used were specific to the year 2018. The remaining settings for the CDBs are documented in the 2017 NEI TSD. To create the emission factors, MOVES was run separately for each representative county and fuel month for each temperature bin needed for the calendar year 2018. The MOVES results were post-processed into CSV-formatted emission factor tables that can be read by SMOKE-MOVES.

California uses their own emission model, EMFAC, which uses emission inventory codes (EICs) to characterize the emission processes instead of SCCs. EPA had a 2016v1 platform-based set of emissions for 2023. EPA interpolated between 2017 and 2023 to calculate the 2018 onroad emissions for California. 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. The California inventory had CAPs only and did not have NH3 or refueling. The EPA added NH_3 to the CARB inventory by using the state total NH_3 from MOVES and allocating it at the county level based on CO. Refueling emissions were projected from the 2017 NEI using county total refueling VOC from EQUATES 2017 and the 2018 MOVES3 onroad run for CA. CARB VOCs were speciated to VOC HAPs using MOVES VOC speciation. All other HAPs (e.g., metals and PAHs) are from MOVES.

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 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. The ratios were calculated for each county/SCC/pollutant combination based on the California onroad emissions inventory. 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 MOVES3 model. The inputs to spatial apportionment factors in MOVES3 were updated to be consistent with those developed for the 2016v1 platform. MOVES3 was used for all states other than California, which uses their own model, and the Texas Commission on Environmental Quality (TCEQ), which provided their own emissions. California nonroad emissions were provided by the California Air Resources Board (CARB) for the 2017 NEI. The 2018 California nonroad emissions were interpolated from the 2017 NEI and a 2023 projection from the 2016v1 modeling platform, with HAP augmentation. The EPA used an existing 2018 interpolation (between 2017 and 2020) for Texas, with HAP augmentation. Canadian nonroad emissions came from the EQUATES 2016/2017 platform and were projected to 2018 using US MOVES-based trends. Mexican nonroad emissions were from the EQUATES 2016 platform and were not projected to 2018 for lack of projection data.

MOVES creates a monthly emissions inventory for criteria air pollutants (CAPs) and a full set of HAPs, plus additional pollutants such as NONHAPTOG and ETHANOL, which are not part of the NEI but are used for speciation. MOVES provides estimates of NONHAPTOG along with the speciation profile code for the NONHAPTOG emission source. This was accomplished by using NHTOG#### as the pollutant code in the Flat File 2010 (FF10) inventory file that can be read into SMOKE, where #### is a speciation profile code. For California and Texas, NHTOG####-VOC and HAP-VOC ratios from MOVES-based emissions were applied to VOC emissions so that VOC emissions can be speciated consistently with other states.

MOVES also provides estimates of $PM_{2.5}$ by speciation profile code for the $PM_{2.5}$ emission source, using PM25_#### as the pollutant code in the FF10 inventory file, where #### is a speciation profile code. To facilitate calculation of PMC within SMOKE, and to help create emissions summaries, an additional pollutant representing total $PM_{2.5}$ called PM25TOTAL was added to the inventory. As with VOC, $PM_{2.5}$_####-PM25TOTAL ratios were calculated and applied to $PM_{2.5}$ emissions in California and Texas so that $PM_{2.5}$ emissions can be speciated consistently with other states.

MOVES outputs emissions data in county-specific databases, and then a post-processing script converted the data into FF10 format. Additional post-processing steps were performed as follows:

- County-specific FF10s were combined into a single FF10 file.

- To reduce the size of the inventory, HAPs that are not needed for air quality modeling, such as dioxins and furans, were removed from the inventory.

- To reduce the size of the inventory further, all emissions for sources (identified by county/SCC) for which total CAP emissions are less than $1*10^{-10}$ were removed from the inventory. The MOVES model attributes a very tiny amount of emissions to sources that are actually zero, for

example, snowmobile emissions in Florida. Removing these sources from the inventory reduces the total size of the inventory by 7%.

- Gas and particulate components of HAPs that come out of MOVES separately, such as naphthalene, were combined.

- VOC was renamed VOC_INV so that SMOKE does not speciate both VOC and NONHAPTOG, which would result in a double count.

- PM25TOTAL, referenced above, was also created at this stage of the process.

- California and Texas emissions from MOVES were deleted, in favor of the CARB and TCEQ data.

- Emissions for airport ground support vehicles (SCCs ending in -8005), and oil field equipment (SCCs ending in -10010), were removed from the inventory at this stage, to prevent a double count with the airports and np_oilgas sectors, respectively.

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. Typically, in the NEI, yard locomotive emissions are split between the nonpoint and point categories, but for this study, all yard locomotive emissions are represented as point sources and included in the ptnonipm sector.

This study uses a new 2017 rail inventory developed for the 2017 NEI by the Lake Michigan Air Directors Consortium (LADCO) and the State of Illinois with support from various other states. Class I railroad emissions are based on confidential link-level line-haul activity GIS data layer maintained by the Federal Railroad Administration (FRA). In addition, the Association of American Railroads (AAR) provided national emission tier fleet mix information. Class II and III railroad emissions are based on a comprehensive nationwide GIS database of locations where short line and regional railroads operate. Passenger rail (Amtrak) emissions follow a similar procedure as Class II and III, except using a database of Amtrak rail lines. Yard locomotive emissions are based on a combination of yard data provided by individual rail companies, and by using Google Earth and other tools to identify rail yard locations for rail companies which did not provide yard data. Information on specific yards were combined with fuel use data and emission factors to create an emissions inventory for rail yards. More detailed information on the development of the 2017 rail inventory for this study is available in the 2017 NEI TSD. The 2017 inventory was projected to 2018 using activity-based factors. Pollutant-specific factors were applied on top of the activity-based changes for the Class I rail. Some corrections to spatial surrogates were also corrected for the 2018 modeling platform as described in section 3.3.

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 based on the 2017 NEI. 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. For more information on CMV sources in the 2017 NEI, see Section 4.21 of the 2017 NEI 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 hourly gridded point sources with stack parameters that should result in them being placed in layer 1. The C1C2 were projected from 2017 to 2018, based on the growth from 2016 to 2017, which resulting in a small adjustment factor of 1.012, which was applied across the board to the 2017 NEI.

The Category 3 CMV vessels in the cmv_c3 sector use residual oil when they are outside of emission control areas. The emissions in the cmv_c3 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. The 2018 cmv_c3 sector uses AIS derived 2017 NEI emissions in a gridded point source format. Emissions from the Emissions Control Area-International Marine Organization (ECA-IMO)-based C3 CMV are used for waters not covered by the AIS selection (portions of FIPS code 98001).

The 2017 NEI C3 inventory was developed as an hourly point inventory from 5 minute-resolution Automated Identification System (AIS) transponder data which had emissions computed from it. Plume rise calculations for C3 vessels are computed when the sources are modeled by SMOKE and CMAQ. To develop the point inventory, the AIS emissions were aggregated to hourly values by grid cell, port identifier, SCC, and FIPS on the 12 km modeling domain. Release point locations were assigned to the centroid of the corresponding grid cell. Emissions where the source vessel idled in the same location for longer than an hour (hoteling) were apportioned to the subsequent hours from the initial time based on the duration of hoteling. Hoteling was capped at 400 hours and emissions were adjusted down proportionally where a vessel exceeded 400 hours in a single location.

Emissions from vessels that occur within the boundaries of a 2017 NEI port polygon were given a port SCC and assigned the appropriate port shape identifier. All other emissions were assigned an underway SCC and not given a port shape identifier. FIPS were assigned to the 5-minute AIS data using a polygon shapefile of US counties extending into state waters, Canadian provinces extending into provincial waters, Mexican states, and US federal water economic exclusive zones (EEZ).

The Category 3 (C3) CMV emissions were projected from 2017 to 2018 using an EPA report on projected bunker fuel demand (See Table 3-6). The report projects bunker fuel consumption by region out to the year 2030. Bunker fuel usage was used as a surrogate for marine vessel activity. Factors based on the report were used for all pollutants except NOx. Growth factors for NOx emissions were handled separately to account for the phase in of Tier 3 vessel engines.

Table 3-6. Projection Factors for 2017 to 2018 for Category 3 Vessels

Region	NOx	All other pollutants
US East Coast	0.9869	1.0346
US South Pacific	0.9494	1.0153
US North Pacific	0.9926	1.0246
US Gulf of Mexico	0.9910	1.0253
US Great Lakes	1.0051	1.0173

The resulting annual point emissions were converted to an annual point 2010 flat file format (FF10). A set of standard stack parameters were assigned to each release point in the cmv_c3 inventory. The assigned stack height was 65.62 ft, the stack diameter was 2.625 ft, the stack temperature was 539.6 °F, and the velocity was 82.02 ft/s. Hourly emissions were converted to an hourly point 2010 FF10.

In 2014, marine vessels in the North American Emission Control Area (ECA), which extends 200 miles from the shores of North America, Puerto Rico, and the Virgin Islands, met a fuel sulfur standard of 10,000 ppm. On January 1st, 2015, the ECA initiated a fuel sulfur standard which regulated large marine vessels to use fuel with 1,000 ppm sulfur or less. EPA multiplied European Union (EU)[6] C3 emissions factors that include these standards with the entrance and clearance (E&C) calls (that specify the origin and destination of the ship) of the respective years.

The EU emission factors also reflect IMO Tier 3 NOx regulations that apply to engines installed on ships constructed (i.e., keel is laid) on or after January 1st, 2016. However, in allotting time for ship building and engine installation, EPA does not expect Tier 3 vessels to be active by December 31st, 2016. The 2017 CMV emissions were computed taking these standards into account

3.2.6 Emissions from Canada, Mexico (othpt, othar, othafdust, othptdust, onroad_can, onroad_mex, ptfire_othna)

The emissions from Canada and Mexico are included as part of the emissions modeling sectors: othpt, othar, othafdust, othptdust, 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), and "ptdust" for point fugitive dust (Canada only).

Emissions in these sectors were taken from the EQUATES 2016 inventories. ECCC provided the following inventories for use in EQUATES 2016 and 2017 modeling, which are described in more detail below:

- Ag livestock and fertilizer, airports in a point source format
- CMV were provided as area sources but converted to point (not currently used)
- Ag fugitive dust, point source format (othptdust sector)
- Other area source dust (othafdust sector)
- Onroad (onroad_can sector)
- Nonroad and rail (othar sector)
- Other area sources (othar sector)

Canadian point sources (othpt) were taken from the EQUATES 2016 inventories, which were built from the ECCC 2016 emission inventory. The othpt sector incudes EGUs, non-EGUs, upstream oil and gas emissions, and agricultural ammonia and VOC. 2016 point source emissions for Mexico were provided by SEMARNAT. The Canadian point source inventory is pre-speciated for the CB6 chemical mechanism. For Canada, agricultural data were originally provided on a rotated 10-km grid for the 2016beta platform. These were smoothed out so as to avoid the artifact of grid lines in the processed emissions. The data were monthly resolution for Canadian agricultural and airport emissions, along with some Canadian point sources, and annual resolution for the remainder of Canada and all of Mexico. Canadian CMV inventories

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[6] http://ec.europa.eu/environment/air/pdf/chapter1_ship_emissions.pdf.

that had been included in this sector in past modeling platforms are now included in the cmv_c1c2 and cmv_c3 sectors as point sources.

Fugitive dust sources of particulate matter emissions excluding land tilling from agricultural activities, were provided by Environment and Climate Change Canada (ECCC) as part of their 2016 emission inventory. Different source categories were provided as gridded point sources and area (nonpoint) source inventories. Gridded point source emissions resulting from land tilling due to agricultural activities were provided as part of the ECCC 2016 emission inventory. The provided wind erosion emissions were removed. The othptdust emissions have a monthly resolution. A transport fraction adjustment that reduces dust emissions based on land cover types was applied to both point and nonpoint dust emissions, along with a meteorology-based (precipitation and snow/ice cover) zero-out of emissions when the ground is snow covered or wet. The EQUATES 2016 inventory was used as-is with 2018 meteorology applied.

The onroad emissions for Canada and Mexico are in the onroad_can and onroad_mex sectors, respectively. Emissions for Canada and Mexico come from the EQUATES 2016 (2016 was the latest year provided by Environment and Climate Change Canada (ECCC)), except for onroad and nonroad. The EPA projected Canada onroad and nonroad from 2016 to 2018 using US MOVES-based trends. Mexican emissions were mostly left as they were in the EQUATES 2016 inventories.

ECCC provided year 2016 Canada province, and in some cases sub-province, resolution emissions from for nonpoint and nonroad sources (othar). The nonroad sources were monthly while the nonpoint and rail emissions were annual. For Mexico, year 2016 Mexico nonpoint and nonroad inventories at the municipio resolution provided by SEMARNAT were used. All Mexico inventories were annual resolution.

Annual point source 2018 day-specific wildland fire emissions for Mexico, Canada, Central America, and Caribbean nations were developed from a combination of the Fire Inventory from NCAR (FINN) daily fire emissions and fire data provided by Environment Canada when available. Only CAP emissions are provided in the ptfire_othna sector inventories. For FINN fires, listed vegetation type codes of 1 and 9 are defined as agricultural burning, all other fire detections and assumed to be wildfires. All wildland fires that are not defined as agricultural are assumed to be wild fires rather than prescribed. FINN fire detects less than 50 square meters (0.012 acres) are removed from the inventory. The locations of FINN fires are geocoded from latitude and longitude to FIPS code.

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 4.8.1 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 3-7 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 3-7. Key emissions modeling steps by sector

Platform sector	Spatial	Speciation	Inventory resolution	Plume rise
afdust_adj	Surrogates	Yes	annual	
Airports	Point	Yes	annual	none
Beis	Pre-gridded land use	in BEIS3.7	computed hourly	
cmv_c1c2	Point	Yes	hourly	in-line
cmv_c3	Point	Yes	hourly	in-line
livestock	Surrogates	Yes	annual	
Nonpt	Surrogates & area-to-point	Yes	annual	
Nonroad	Surrogates	Yes	monthly	
np_oilgas	Surrogates	Yes	annual	
Onroad	Surrogates	Yes	monthly activity, computed hourly	
onroad_ca_adj	Surrogates	Yes	monthly activity, computed hourly	
onroad_can	Surrogates	Yes	monthly	
onroad_mex	Surrogates	Yes	monthly	
othafdust_adj	Surrogates	Yes	annual	
othptdust_adj	Point	Yes	monthly	none
Other	Surrogates	Yes	annual & monthly	
Othpt	Point	Yes	annual & monthly	in-line
Ptagfire	Point	Yes	daily	in-line
pt_oilgas	Point	Yes	annual	in-line
ptegu	Point	Yes	daily & hourly	in-line
ptfire-rx	Point	Yes	daily	in-line
ptfire-wild	Point	Yes	daily	in-line
ptfire_othna	Point	Yes	daily	in-line
ptnonipm	Point	Yes	annual	in-line
rail	Surrogates	Yes	annual	
rwc	Surrogates	Yes	annual	
vcp	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 stack parameters and the hourly emissions in the SMOKE output files for each emissions sector. The height of the plume rise determines the model layer into which the emissions are placed. All of these particular sectors only have "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 fire emissions are treated differently in CMAQ. After plume rise is applied, there are emissions in every layer from the ground up to the top of the plume. The emissions in the airports and othptdust sectors are all low-level emissions, and so in-line emissions files are not created for these two sectors. Instead, all airports and othptdust emissions are output to gridded emissions files, same as if airports and othptdust were area source sectors.

SMOKE has the option of grouping sources so that they are treated as a single stack when computing plume rise. For this 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 3-3, but the air quality model was run on the smaller 12-km domain (12US2). 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.
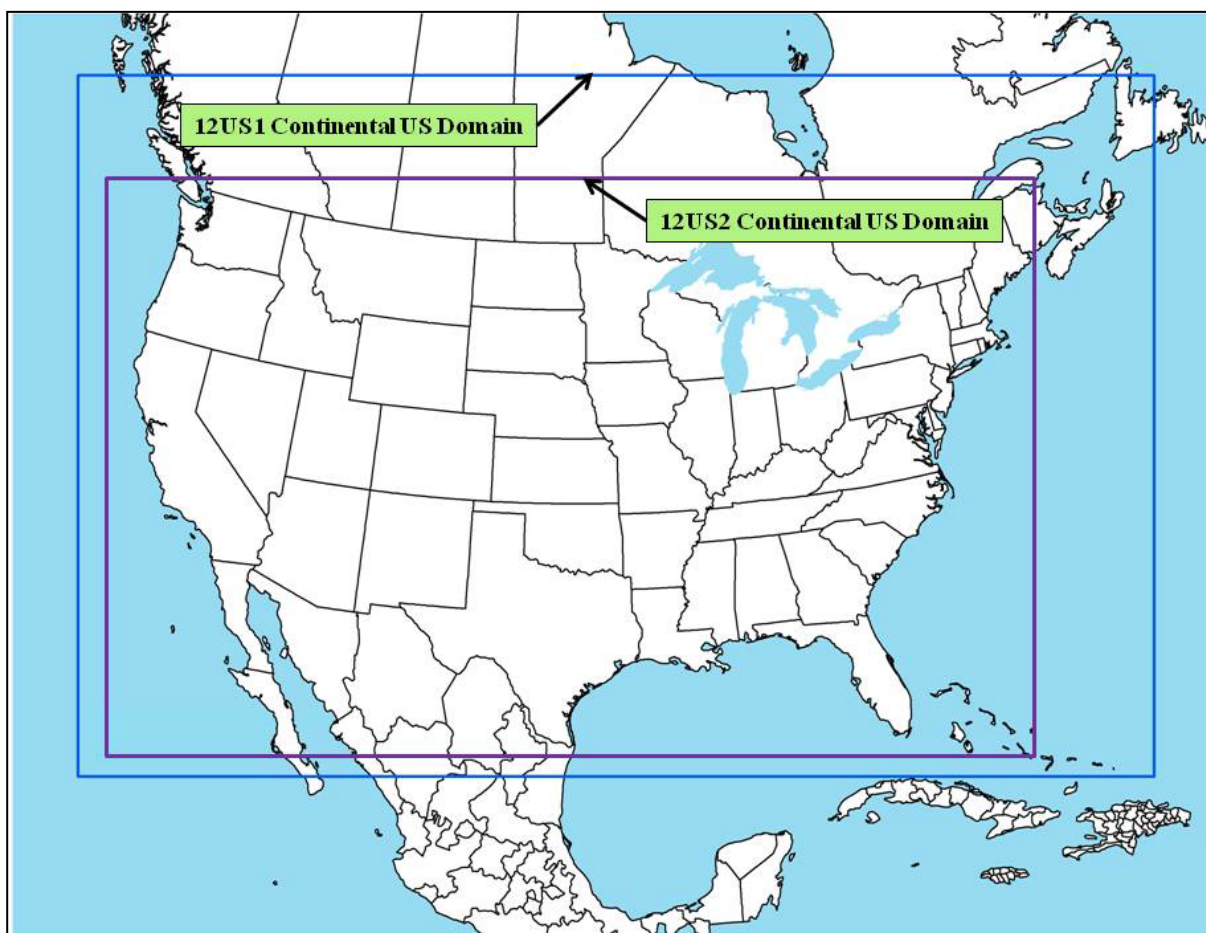
Figure 3-3. CMAQ Modeling Domain

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 platform is the CB6 mechanism (Yarwood, 2010). We used an updated version of CB6 that we refer to as "CB6R3AE7" which includes four new species that were not in the previous version of CB6: AACD, FACD, APIN, and IVOC. This mapping uses a new systematic methodology for mapping low volatility compounds. Compounds with very low vapor pressure are mapped to model species NVOL and intermediate volatility compounds are mapped to a species called IVOC. In previous mappings, some of these low vapor pressure compounds were mapped to CB6 species. The mechanism and mapping are described in more detail in a memorandum describing the mechanism files supplied with the Speciation Tool, the software used to create the CB6 profiles used in SMOKE. It should be noted that the onroad mobile sector does not use this newer mapping because the speciation is done within MOVES and the mapping change was made after MOVES had been run.

This platform generates the PM$_{2.5}$ model species associated with the CMAQ Aerosol Module version 7 (AE7) which has the same PM$_{2.5}$ model species as version 6 (AE6). The AE7 mechanism is built on the AE6 and identical in terms of model species and mechanism definition but requires that alpha-pinene (APIN) be separate from all other monoterpenes (TERP) and not included in TERP to avoid double counting. Table 3-8 lists the model species produced by SMOKE in the platform used for this study.

Table 3-8. Emission model species produced for CB6R3AE7 for CMAQ

Inventory Pollutant	Model Species	Model species description
Cl₂	CL2	Atomic gas-phase chlorine
HCl	HCL	Hydrogen Chloride (hydrochloric acid) gas
CO	CO	Carbon monoxide
NOₓ	NO	Nitrogen oxide
	NO2	Nitrogen dioxide
	HONO	Nitrous acid
SO₂	SO2	Sulfur dioxide
	SULF	Sulfuric acid vapor
NH₃	NH3	Ammonia
	NH3_FERT	Ammonia from fertilizer
VOC	AACD	Acetic acid
	ACET	Acetone
	ALD2	Acetaldehyde
	ALDX	Propionaldehyde and higher aldehydes
	APIN	alpha-Pinene
	BENZ	Benzene
	CH4	Methane
	ETH	Ethene
	ETHA	Ethane
	ETHY	Ethyne
	ETOH	Ethanol
	FACD	Formic acid
	FORM	Formaldehyde
	IOLE	Internal olefin carbon bond (R-C=C-R)
	ISOP	Isoprene
	IVOC	Intermediate volatility organic compounds
	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
PM₁₀	PMC	Coarse PM > 2.5 microns and ≤ 10 microns
PM₂.₅	PEC	Particulate elemental carbon ≤ 2.5 microns

Inventory Pollutant	Model Species	Model species description
	PNO3	Particulate nitrate ≤ 2.5 microns
	POC	Particulate organic carbon (carbon only) ≤ 2.5 microns
	PSO4	Particulate Sulfate ≤ 2.5 microns
	PAL	Aluminum
	PCA	Calcium
	PCL	Chloride
	PFE	Iron
	PK	Potassium
	PH2O	Water
	PMG	Magnesium
	PMN	Manganese
	PMOTHR	PM$_{2.5}$ not in other AE6 species
	PNA	Sodium
	PNCOM	Non-carbon organic matter
	PNH4	Ammonium
	PSI	Silica
	PTI	Titanium
Sea-salt species (non – anthropogenic) [7]	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 5.1 database (https://www.epa.gov/air-emissions-modeling/speciate), which is the EPA's repository of TOG and PM speciation profiles of air pollution sources. The SPECIATE database development and maintenance is a collaboration involving the EPA's Office of Research and Development (ORD), Office of Transportation and Air Quality (OTAQ), and the Office of Air Quality Planning and Standards (OAQPS). 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 of the speciation approach for this study are listed here and described further in the subsections below:

- Use of the CBR3AE7 mechanism
- Non-methane organic gases (NMOG), which are total organic gases with methane subtracted from it, is included as a pollutant in the emissions output files to assist with the use of these data with future versions of the CMAQ model.
- Several new VOC and PM$_{2.5}$ profiles slated for the next version of SPECIATE were used.
- PM$_{2.5}$ and VOC speciation process for nonroad mobile use profiles assigned within MOVES3 (which outputs the emissions with those assignments).
- Some Canadian point source inventories are provided from Environment Canada as pre-speciated emissions, and not all CB6 species were provided; missing species were supplemented by speciating total VOC.
- A GSPRO_COMBO file was used for Canada to account for ethanol mixes in Canadian gasoline.

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[7] These emissions are created outside of SMOKE.

Speciation profiles and cross-references for this study platform are available in the set SMOKE input files for the 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 study.

For onroad mobile sources, speciation is done in MOVES, to allow for profiles that vary by model year, which is not part of the SCC code, to be used. Therefore, cross-references or emissions summaries by profile for onroad mobile sources are not provided. These profiles are documented in a MOVES technical report on speciation (EPA, 2020).

A number of speciation profiles for VOC and PM$_{2.5}$ that had been added in SPECIATE 5.1 were used. In addition, we profile assignments were updated to incorporate data provided by states or to correct errors in previous assignments.

For PM$_{2.5}$ the following profile updates were made for the 2017 platform:

- Corrected the wildfire and prescribed fire profile due to error in compositing (the previous profile included creosote in the average)
- Updated the profile for aircraft
- Corrected several profile assignments for the petroleum industry

For PM$_{2.5}$ the following profile updates were made for the 2018 platform:

- Changed the "Heat Treating" profile to the profile code to 91123 which is the actual Heat Treating profile.
- For 2801500250, changed to profile SUGP02 (new sugar cane burning profile).
- For 30400740, changed to profile 95475.
- Added new fire profiles from Assign_Amara_Fire_PM_Profiles_ModelingPlatform.xlsx. All US states (not DC/HI/PR/VI) now use one of the new profiles for all fire SCCs, including grassland fires. The profiles themselves aren't entirely state-specific; there are 4 representative states for forest fires and 2 representative states for grass fires, and all states are mapped to one of the four representative forest states and one of the two representative grass states in the Amara workbook. The GSREFs still have a non-FIPS-specific assignment to the previous profile 3766AE6 which will be used outside the US.
- Assignments for new PM SCCs in the 2018 point inventory were included.

For VOC the following profile updates were made for the 2017 platform:

- Volatile consumer products - new methods to estimate emissions of Volatile Organic Compounds (VOC) and associated Hazardous Air Pollutants (HAPs) from Volatile Chemical Products (VCPs) were used in this 2018 modeling platform. The new methods result in improved emissions estimates for the nonpoint (county-wide) solvent emissions. The new emissions method results in improved VOC and HAP estimates for nonpoint categories of coatings, pesticides, adhesives and sealants, oil & gas exploration solvent use, dry cleaning, printing inks, cleaning products, personal care products, and other miscellaneous solvent uses. See section 3.2.1.4 for more details.

- Oil and Gas –incorporated region-specific profiles or updated assignments
  - Used county-specific profiles gas for several Wyoming counties developed from data provided by the Wyoming DEQ
  - Used Willison Basin gas composition data, separate profiles for the Montana and North Dakota portions of the basin, based on data developed by the Western Regional Air Partnership WRAP
  - Used Central Montana Uplift area gas composition data, based on data developed by the WRAP
  - Updated Uinta basin profile assignments (based on data provided by Utah)
  - Used Utah and Wyoming oil and gas produced water pond profiles
  - Profile assignments (by county and SCC) for nonpoint oil and gas sources that account for the portion of VOC estimated to come from flares were based on results from the Oil and Gas estimation tool run for the 2017 NEI.
  - Updated profile assignment for miscellaneous engines to use internal combustion engine natural gas profile
- Commercial Marine vessel – changed profile assignment to an existing Pre-Tier 1 nonroad diesel profile because the previous profile was missing key species (aldehydes)
- Livestock – updated profile assignments
- Agricultural burning – updated profiles for rice straw and wheat straw burning, and used new sugar cane burning profile

For VOC the following cross reference updates updates were made for the 2018 platform:
- Changed all 8746 to G8746 (Profile name: Rice Straw and Wheat Straw Burning Composite of G4420 and G4421)
- Changed 2104008230/330 from 1084 to 4642 to match all other RWC SCCs (corrections_changes .docx said 4462 but this was an obvious typo and should be 4642)
- Changed all SCCs in the Karl Seltzer VCPy inventory to use the VCPy speciation profiles
- Changed 2680001000 from 0000 to G95241TOG
- Uinta Basin oil/gas profiles:
  - Replaced profile 95417 with either UTUBOGC (2310010300, 2310011500, 2310111401, 2310010700, 2310010400, 31000107) or UTUBOGD (other SCCs)
  - Replaced profile 95418 with UTUBOGF
  - Replaced profile 95419 with UTUBOGE

- PA gas profiles: Replaced all 8949 with PAGAS01 (FIPS 42059 only), PAGAS02 (FIPS 42019 only), PAGAS03 (FIPS 42125 only). To do this, we first replaced existing county-specific 8949 profiles with the new PAGAS profiles for these three counties in the ERG COMBO GSREF. This covered 5 SCCs. For all SCCs other than those 5 SCCs, where the national profile assignment is 8949. New county-specific profile assignments were made to the appropriate PAGAS profile for each of the three counties, added to the Ramboll basin specific GSREF (since that GSREF is also county-specific and not combo).

- Colorado 2310030300: Set Archuleta/La Plata to SUIROGWT (counties are in Southern Ute reservation), rest of Colorado to DJTFLR95

- Colorado 2310030220: Set to DJTFLR95 (formerly FLR99)

- Colorado 2310021010: Set Archuleta/La Plata to SUIROGCT (counties are in Southern Ute reservation), rest of Colorado to 95398

- Changed 2310000551 (CBM produced water) to a new profile, CBMPWWY. Speciation Tool inputs for this profile tool run by GDIT. Documentation: Profiles are means from WY tests in SPECIATE, newly composited. Reference: https://doi.org/10.1016/j.scitotenv.2017.11.161 Reference: Lyman, Seth N.; Mansfield, Marc L.; Tran, Huy N. Q.; Evans, Jordan D.; Jones, Colleen; O'Neil, Trevor; Bowers, Ric; Smith, Ann; and Keslar, Cara, "Emissions of organic compounds from produced water ponds I: Characteristics and speciation" (2018). Chemistry and Biochemistry Faculty Presentations. Paper 154. Contact: Art Diem and Jeff Vukovich of the EPA's Office of Air Quality Planning and Standards (OAQPS)

- Assignments for new VOC SCCs in the 2018 point inventory were included along with changes to VOC profiles for 16 point SCCs.

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

The integration of HAP VOC with VOC is a feature available in SMOKE for all inventory formats, including PTDAY (the format used for the ptfire and ptagfire sectors). The ability to use integration with

the PTDAY format was made available in the version of SMOKE used for the v7.1 platform, and this new feature is used for this particular study because the ptfire and ptagfire inventories for this study include HAPs. 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[8]). 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.[9] SMOKE computes NONHAPTOG and then applies the speciation profiles to allocate the NONHAPTOG to the other air quality model VOC species not including the integrated HAPs. After determining if a sector is to be integrated, if all sources have the appropriate HAP emissions, then the sector is considered fully integrated and does not need a NHAPEXCLUDE file. If, on the other hand, certain sources do not have the necessary HAPs, then an NHAPEXCLUDE file must be provided based on the evaluation of each source's pollutant mix. The EPA considered CAP-HAP integration for all sectors in determining whether sectors would have full, no, or partial integration (see Figure 3-4). 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.

Figure 3-4 illustrates the integrate and no-integrate processes for U.S. Sources. Since Canada and Mexico inventories do not contain HAPs, we use the approach of generating the HAPs via speciation, except for Mexico onroad mobile sources where emissions for integrate HAPs were available.

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

In SMOKE, the INVTABLE allows the user to specify the particular HAPs to integrate. Two different INVTABLE files are used for different sectors of the platform. For sectors that had no integration across the entire sector (see Table 3-9), 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 for those sectors. Where applied, 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.

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[8] 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.

[9] 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.
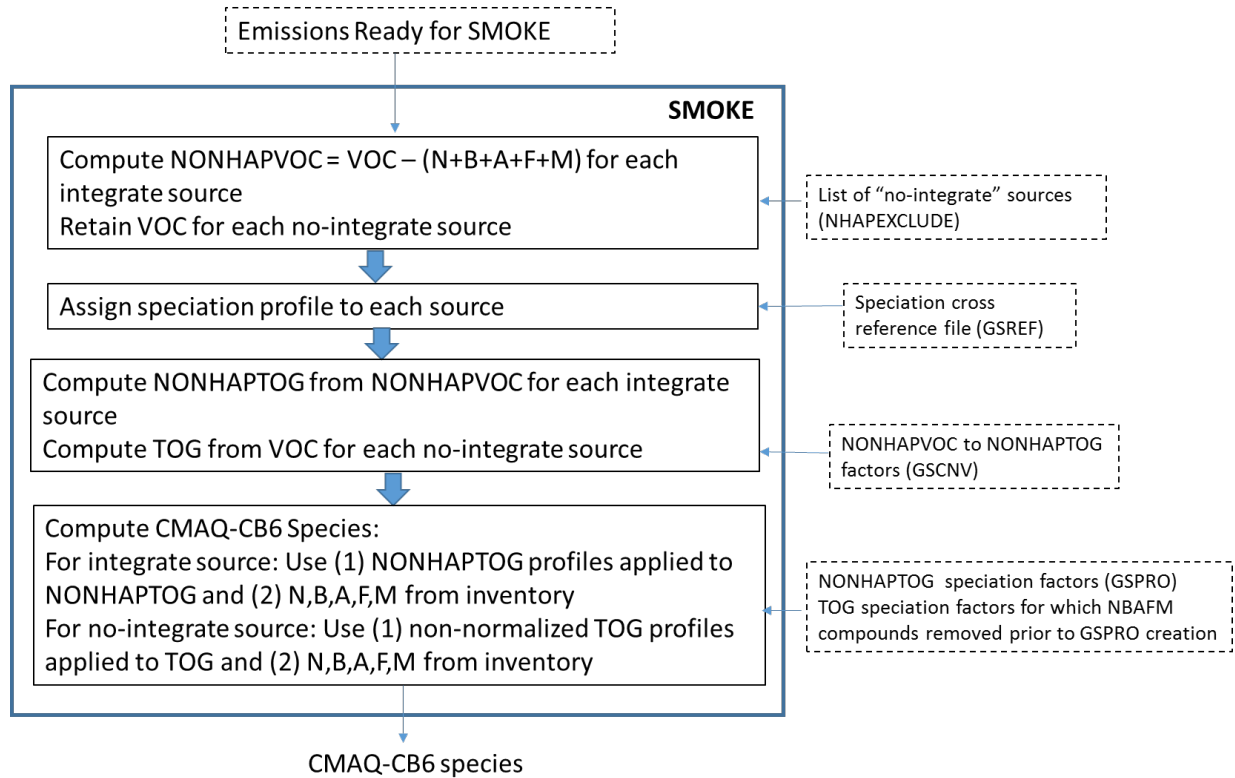
Figure 3-4. Process of integrating NBAFM with VOC for use in VOC Speciation

Table 3-9. Integration status of naphthalene, benzene, acetaldehyde, formaldehyde and methanol (NBAFM) for each platform sector

Platform Sector	Approach for Integrating NEI emissions of Naphthalene (N), Benzene (B), Acetaldehyde (A), Formaldehyde (F) and Methanol (M)
afdust	N/A – sector contains no VOC
airports	No integration, use NBAFM from inventory
beis	N/A – sector contains no inventory pollutant "VOC"; but rather specific VOC species
cmv_c1c2	No integration, create NBAFM from VOC speciation
cmv_c3	No integration, create NBAFM from VOC speciation
livestock	Partial integration (NBAFM)
nonpt	Partial integration (NBAFM)
nonroad	Full integration (internal to MOVES elsewhere)
np_oilgas	Partial integration (NBAFM)
onroad	Full integration (internal to MOVES elsewhere)
onroad_can	No integration, no NBAFM in inventory, create NBAFM from speciation
onroad_mex	Full integration (internal to MOVES-Mexico); however, MOVES-MEXICO speciation was for CB6R3AE6
othafdust	N/A – sector contains no VOC
othar	No integration, no NBAFM in inventory, create NBAFM from VOC speciation
othpt	No integration, no NBAFM in inventory, create NBAFM from VOC speciation
othptdust	N/A – sector contains no VOC
pt_oilgas	No integration, use NBAFM from inventory

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Platform Sector	Approach for Integrating NEI emissions of Naphthalene (N), Benzene (B), Acetaldehyde (A), Formaldehyde (F) and Methanol (M)
ptagfire	Full integration (NBAFM)
ptegu	No integration, use NBAFM from inventory
ptfire	Partial integration (NBAFM)
ptfire_othna	No integration, no NBAFM in inventory, create NBAFM from VOC speciation
ptnonipm	No integration, use NBAFM from inventory
rail	Full integration (NBAFM)
rwc	Full integration (NBAFM)
vcp	Partial integration (NBAFM)

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, VOC speciation is done fully within MOVES 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 CB6R3AE7 mechanism, so no additional species needed to be added after SMOKE-MOVES processing. For nonroad mobile, speciation is partially done within MOVES such that MOVES does not need to be run for a specific chemical mechanism. For nonroad, MOVES outputs emissions of HAPs and NONHAPTOG were split by speciation profile. Taking into account that integrated species were subtracted out by MOVES already, the appropriate speciation profiles are then applied within 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 2017 platform, GSPRO_COMBO is still used for certain gasoline-related stationary sources nationwide. GSPRO_COMBO is no longer needed for nonroad sources 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.

In Canada, ECCC provided estimates of ethanol mixes by Canadian province. These estimates were used to develop a GSPRO_COMBO for Canadian gasoline onroad emissions. For example, a province where the average ethanol mix is 6% would have 60% E10 speciation and 40% E0 speciation. A 10% ethanol mix would imply 100% E10 speciation. In Mexico, only E0 speciation profiles are used, but the GSPRO_COMBO feature is still used in Mexico for inventories where VOC emissions are not explicitly defined by mode (e.g., exhaust versus evaporative). Here, the GSPRO_COMBO specifies a mix of exhaust and evaporative speciation profiles. Using the GSPRO_COMBO to split total VOC into exhaust and evaporative components is no longer necessary for Canadian mobile sources, whose inventories include the mode in the pollutant, or for Mexico onroad sources, where VOC speciation is calculated by the MOVES model. The GSPRO_COMBO is still used for Mexican nonroad sources which do not have modes in the inventory.

The newer combo method for combining profiles that is available in SMOKE4.5 and later versions is used in this platform and allows multiple profiles to be combined by pollutant, state and county (i.e., state/county FIPS code), and SCC. This is used specifically for the np_oilgas sector because SCCs include both controlled and uncontrolled oil and gas operations which use different profiles. The underlying data which defines the profile splits for oil and gas was updated for this study.

Speciation profiles for use with BEIS are not included in SPECIATE. BEIS includes a species Sequiterpenes (SESQ) that was mapped to the CMAQ specie SESQT. The profile code associated with BEIS profiles for use with CB6 was "BC6E7."

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. MOVES produces speciated NO, NO2, and HONO by source, including emission factors for these species in the emission factor tables used by SMOKE-MOVES. Within MOVES, the HONO fraction is a constant 0.008 of NO_X. The NO fraction varies by heavy duty versus light duty, fuel type, and model year, and equals 1 – NO – HONO. For more details on the NO_X fractions within MOVES for onroad, see Exhaust Emission Rates for Heavy-Duty Onroad Vehicles in MOVES3 and Exhaust Emission Rates for Light-Duty Onroad Vehicles in MOVES3.

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

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

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

The following values are used in the above table: The value "all" means that hourly emissions are computed for every day of the year and that emissions potentially have day-of-year variation. The value "week" means that hourly emissions computed for all days in one "representative" week, representing all weeks for each month. This means emissions have day-of-week variation, but not week-to-week variation

within the month. The value "mwdss" means hourly emissions for one representative Monday, representative weekday (Tuesday through Friday), representative Saturday, and representative Sunday for each month. This means emissions have variation between Mondays, other weekdays, Saturdays and Sundays within the month, but not week-to-week variation within the month. The value "aveday" means hourly emissions computed for one representative day of each month, meaning emissions for all days within a month are the same. Special situations with respect to 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, 2018, which is intended to mitigate the effects of initial condition concentrations. The ramp-up period was 10 days (December 22-31, 2017). For all anthropogenic sectors, emissions from December 2018 were used to fill in surrogate emissions for the end of December 2017. In particular, December 2018 emissions (representative days) were used for December 2017. For biogenic emissions, December 2017 emissions were processed using 2017 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 othptdust.

3.3.5.1 Standard Temporal Profiles

Some sectors use straightforward temporal profiles not based on meteorology or other factors. For the ptfire, ptagfire, and ptfire_othna sectors, 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 workday 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.

An update in this 2018 platform was an analysis of monthly temporal profiles for non-EGU point sources in the ptnonipm sector. A number of profiles were found to be not quite flat over the months but were so close to flat that the difference was not meaningful. These profiles were replaced in the cross reference to point instead to the flat monthly profile. The codes for the profiles that were replaced were: 202, 214, 220, 221, 222, 223, 227, 257, 263, 264, 265, 266, 267, 269, 271, 272, 279, 280, 295, 302, 303, 304, 305, 306, 309, 310, 327, 329, 332, and 333.

For the cmv sectors, most of the emissions are computed hourly and not dependent on temporal profiles. For areas that did not use AIS data, C1 and C2 monthly profiles are flat and C3 monthly profiles are highest (but not significantly different from the rest of the year) in the summer.

A monthly temporal profile for freight rail was developed from AAR data for the year 2016 (https://www.aar.org/data-center/rail-traffic-data/) and continues to be used in this study, Monthly Rail Traffic Data, Total Carloads & Intermodal. Passenger trains use a flat monthly profile. Monthly passenger miles data are available; however, it is not known if there is a correlation between passenger miles and actual rail emissions. This is because passenger trains often operate on a fixed schedule, independent of actual passenger traffic. So, it was decided to not apply a monthly profile to passenger train emissions. All sources in the rail sector use a flat profile for both day-of-week and hour-of-day temporalization.

For the ptfire and ptagfire sectors, the inventories are in the daily point fire format, so temporal profiles are only used to go from day-specific to hourly emissions. For ptfire, state-specific hourly profiles were used, with distinct profiles for prescribed fires and wildfires. For ptagfire, the diurnal temporal profile used reflected the fact that burning occurs during the daylight hours. Additional details on these profiles are available in the 2016v1 platform TSD (EPA, 2020b).

For the nonroad sector, while the NEI only stores the annual totals, the modeling platform uses monthly inventories from output from MOVES. For California, CARB's annual inventory was temporalized to monthly using monthly temporal profiles applied in SMOKE by SCC.

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 10 PM and 6 AM 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.

Monthly temporalization of np_oilgas emissions is based primarily on monthly factors from the Oil and Gas Tool (OGT). Factors were specific to each county and SCC. For use in SMOKE, each unique set of factors was assigned a label (OG17_0001 through OG17_6272), and then a SMOKE-formatted ATPRO_MONTHLY and an ATREF were developed. This dataset of monthly temporal factors included profiles for all counties and SCCs in the Oil and Gas Tool inventory. Because we are using non-tool datasets in some states, this monthly temporalization dataset did not cover all counties and SCCs in the entire inventory used for this study. To fill in the gaps in those states, state average monthly profiles for oil, natural gas, and combination sources were calculated from Energy Information Administration (EIA) data and assigned to each county/SCC combination not already covered by the OGT monthly temporal profile dataset. Coal bed methane (CBM) and natural gas liquid sources in those four states were assigned flat monthly profiles where there was not already a profile assignment in the ERG dataset.

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 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

Electric generating unit (EGU) sources matched to ORIS units were temporally allocated to hourly emissions needed for modeling using the hourly CEMS data. Those hourly data were processed through v2.1 of the CEMCorrect tool to mitigate the impact of unmeasured values in the data. An example of before and after the application of the tool is shown in Figure 3-5.
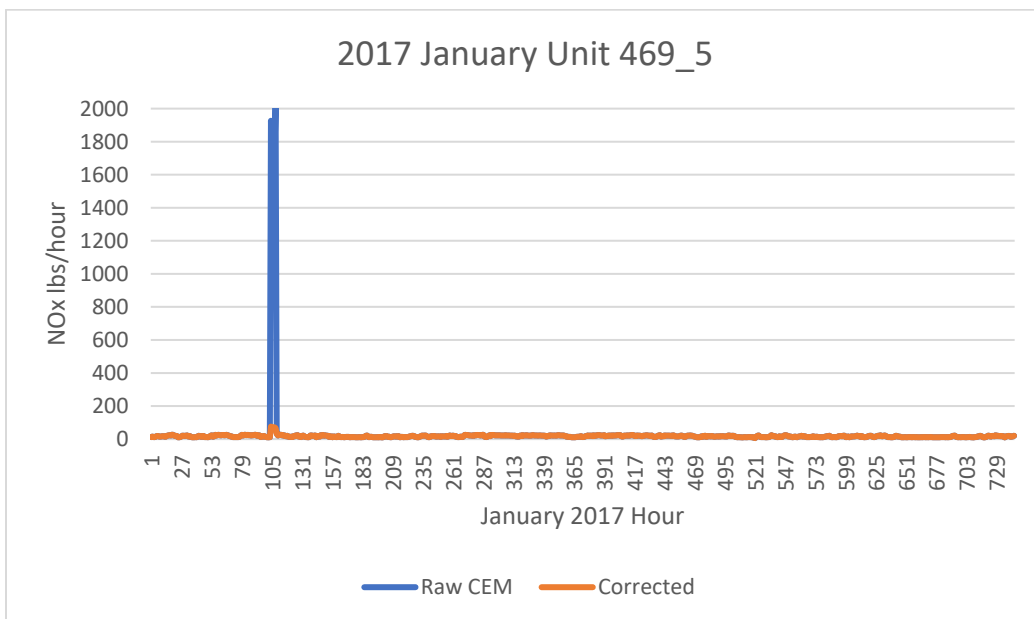

Figure 3-5. Eliminating unmeasured spikes in CEMS data

The region, fuel, and type (peaking or non-peaking) must be identified for each input EGU with CEMS data that are used for generating profiles. The identification of peaking units was done using hourly heat input data from the 2018 base year and the two previous years (2016 and 2017). The heat input was summed for each year. Equation 1 shows how the annual heat input value is converted from heat units (BTU/year) to power units (MW) using the NEEDS v6 derived unit-level heat rate (BTU/kWh). In equation 2 a capacity factor is calculated by dividing the annual unit MW value by the NEEDS v6 unit capacity value (MW) multiplied by the hours in the year. A peaking unit was defined as any unit that had a maximum capacity factor of less than 0.2 for every year (2016, 2017, and 2018) and a 3-year average capacity factor of less than 0.1.

Equation 1. Annual unit power output

$$Annual\ Unit\ Output\ (MW) = \frac{\sum_{i=0}^{8760} \frac{Hourly\ HI}{(BTU)} * 1000 \left(\frac{MW}{kW}\right)}{NEEDS\ Heat\ Rate\ \left(\frac{BTU}{kWh}\right)}$$

Equation 2. Unit capacity factor

$$Capacity\ Factor = \frac{Annual\ Unit\ Output\ (MW)}{NEEDS\ Unit\ Capacity\ \left(\frac{MW}{h}\right) * 8760\ (h)}$$

Input regions were determined from one of the eight EGU modeling regions based on multi-jurisdictional planning organization (MJO) and climate regions. Regions were used to group units with similar climate-based load demands. Region assignment is made on a state level, where all units within a state were assigned to the appropriate region as shown in Figure 3-6. Unit fuel assignments were made using the primary NEEDS v6 fuel. Units fueled by bituminous, subbituminous, or lignite are assigned to the coal fuel type. Natural gas units were assigned to the gas fuel type. Distillate and residual fuel oil were assigned to the oil fuel type. Units with any other primary fuel were assigned the "other" fuel type. Currently there is a possible region, fuel, and type group maximum of 64 based on 8 regions, 4 fuels, and two types (peaking and non-peaking).

The daily and diurnal profiles were calculated for each region, fuel, and peaking type group from the 2016 CEM heat input values. The heat input values were summed for each input group to the annual level at each level of temporal resolution: monthly, month-of-day, and diurnal. The sum by temporal resolution value is then divided by the sum of annual heat input in that group to get a set of temporalization factors. Diurnal factors were created for both the summer and winter seasons to account for the variation in hourly load demands between the seasons. For example, the sum of all hour 1 heat input values in the group was divided by the sum of all heat inputs over all hours to get the hour 1 factor. Each grouping contained 12 monthly factors, up to 31 daily factors per month, and two sets of 24 hourly factors. The profiles were weighted by unit size where the units with more heat input have a greater influence on the shape of the profile. Composite profiles were created for each region and type across all fuels as a way to provide profiles for a fuel type that does not have hourly CEM data in that region. Figure 3-7 shows peaking and non-peaking daily temporal profiles for the gas fuel type in the LADCO region. Figure 3-8 shows the diurnal profiles for the coal fuel type in the Mid-Atlantic/Northeast Visibility Union (MANE VU) region.
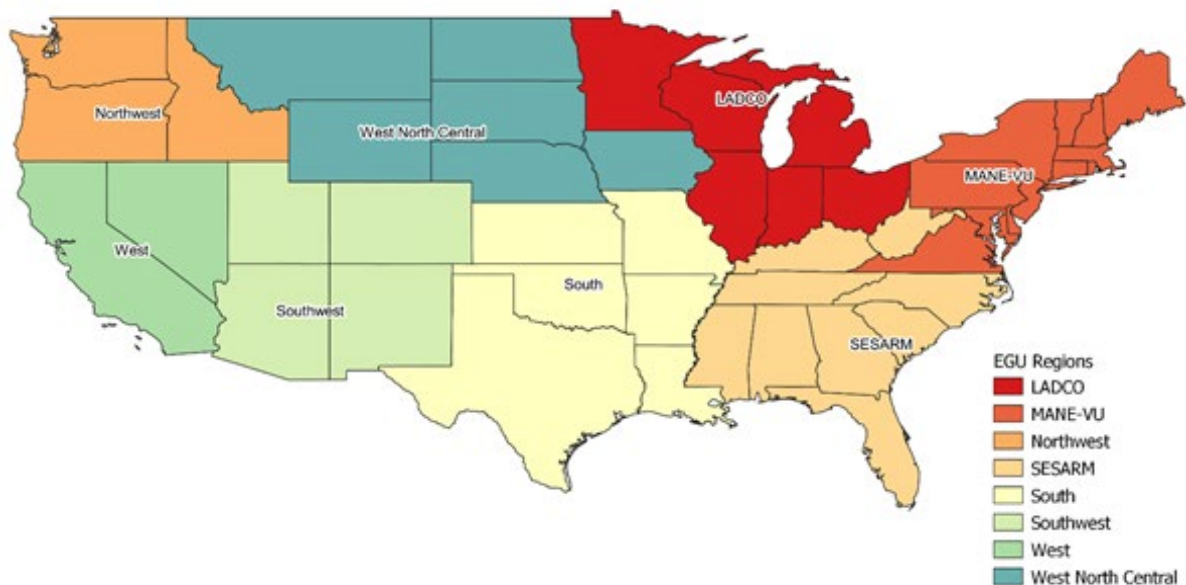

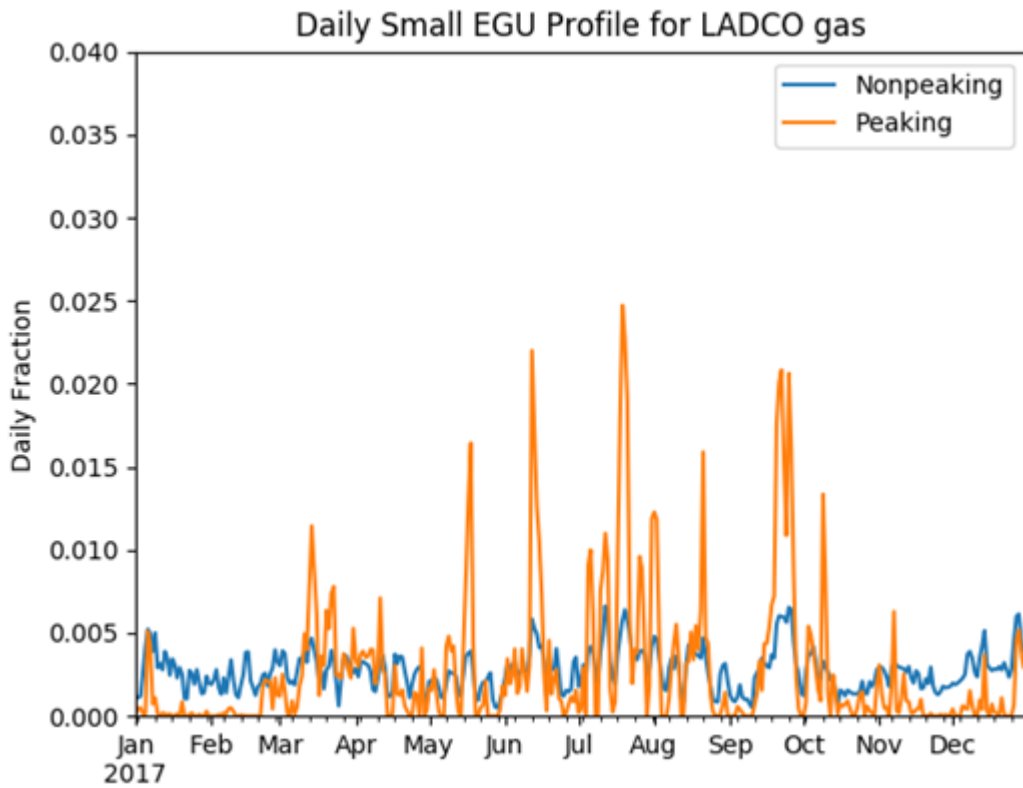**Figure 3-6. Small EGU Temporal Profile Regions**

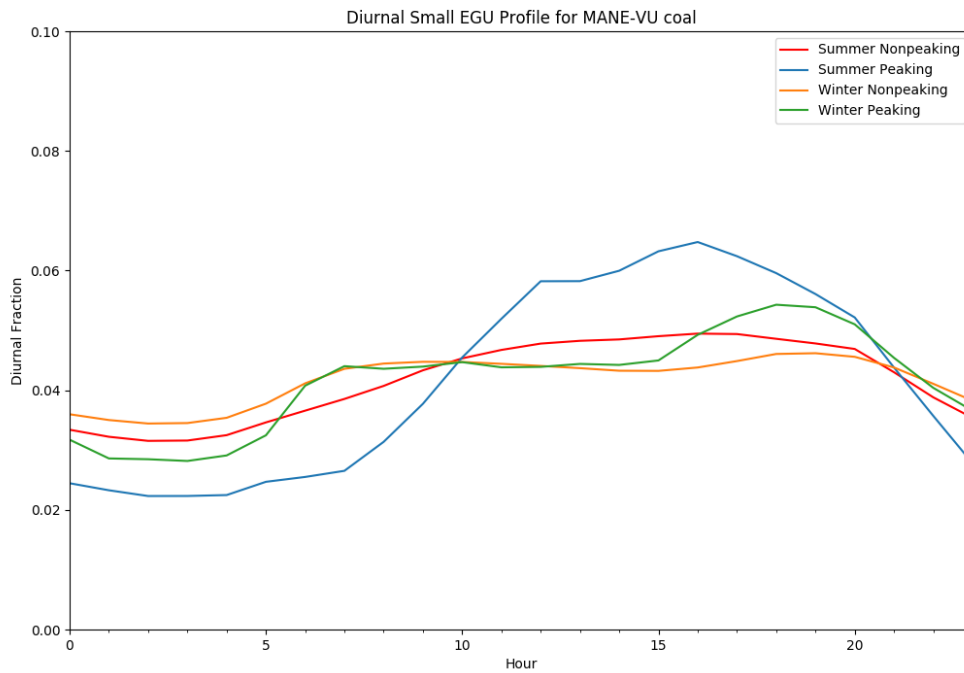**Figure 3-7. Example Daily Temporal Profiles for the LADCO region and Gas Fuel Type**

Figure 3-8. Example Diurnal Profile for MANE-VU Region and Coal Fuel Type

SMOKE uses a cross-reference file to select a monthly, daily, and diurnal profile for each source. For the 2018 platform, the temporal profiles were assigned in the cross-reference at the unit level to EGU sources without hourly CEM data. An inventory of all EGU sources without CEMS data was used to identify the region, fuel type, and type (peaking/non-peaking) of each source. As with the input unit the regions are assigned using the state from the unit FIPS. The fuel is assigned by SCC to one of the four fuel types: coal, gas, oil, and other. A fuel type unit assignment is made by summing the VOC, NO_X, $PM_{2.5}$, and SO_2 for all SCCs in the unit. The SCC that contributed the highest total emissions to the unit for selected pollutants was used to assign the unit fuel type. Peaking units were identified as any unit with an oil, gas, or oil fuel type with a NAICS of 22111 or 221112. Some units may be assigned to a fuel type within a region that does not have an available input unit with a matching fuel type in that region. These units without an available profile for their group were assigned to use the regional composite profile. Municipal waste combustors (MWC) and cogeneration units were identified using the NEEDS primary fuel type and cogeneration flag, respectively, from the NEEDS v6 database.

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 a 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 this platform, meteorological-based temporalization was used for portions of the rwc sector and for the entirety of 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 https://www.cmascenter.org/smoke/documentation/4.6/html/ch05s03s05.html, respectively.

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

Figure 3-9 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.
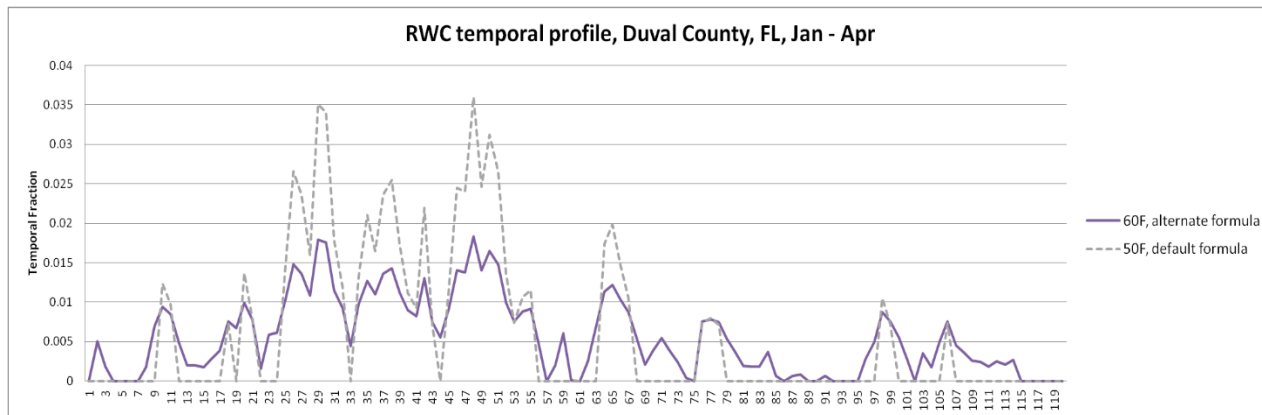

Figure 3-9. Example of RWC temporalization using a 50 ˚F versus 60˚F threshold

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, chimeneas, etc.)" (i.e., "recreational RWC", SCC=21040087000) do not use the same meteorological-based temporalization as the rest of the rwc sector, because meteorological-based temporalization did not agree with observations for how these appliances are used. For hydronic heaters, 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 3-10 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 3-11. 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.

The 2017 NEI includes two new hydronic heater SCCs, 2104008620 (indoor hydronic heaters) and 2104008630 (pellet-fired hydronic heaters). Both of these SCCs use the same monthly, weekly, and diurnal temporal profiles as OHHs.
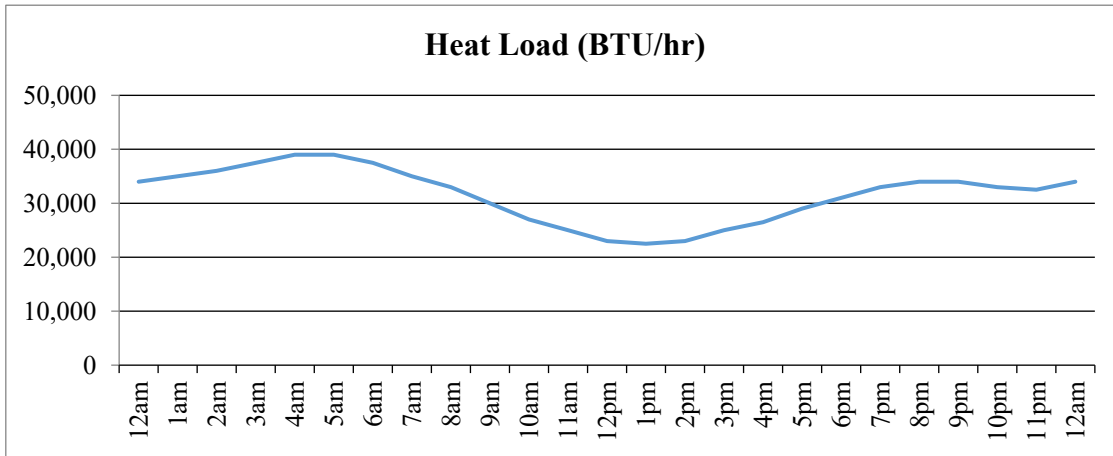
Heat Load (BTU/hr)

Figure 3-10. Diurnal profile for OHH, based on heat load (BTU/hr)

Monthly Temporal Activity for OHH & Recreational RWC
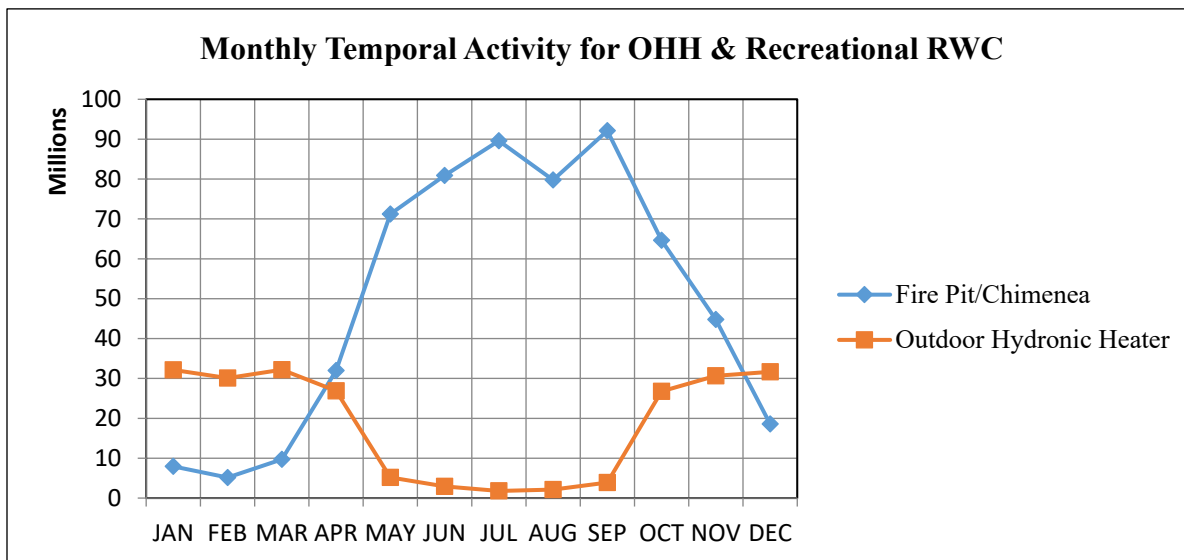
Figure 3--11. Annual-to-month temporal profiles for OHH and recreational RWC

For the ag sector, agricultural GenTPRO temporalization was applied to both livestock and fertilizer emissions, and to all pollutants within the ag sector, not just NH_3. This is a change from the 2014v7.0 modeling platform, in which agricultural GenTPRO temporalization was only applied to livestock NH_3 sources. 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 NH_3 emission variations from livestock as a function of ambient temperature, aerodynamic resistance, and wind speed. The equations are:

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

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

where

- $PE_{i,h}$ = Percentage of emissions in county i in hour h
- $E_{i,h}$ = Emission rate in county i in hour h
- $T_{i,h}$ = Ambient temperature (Kelvin) in county i in 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 3-12 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.
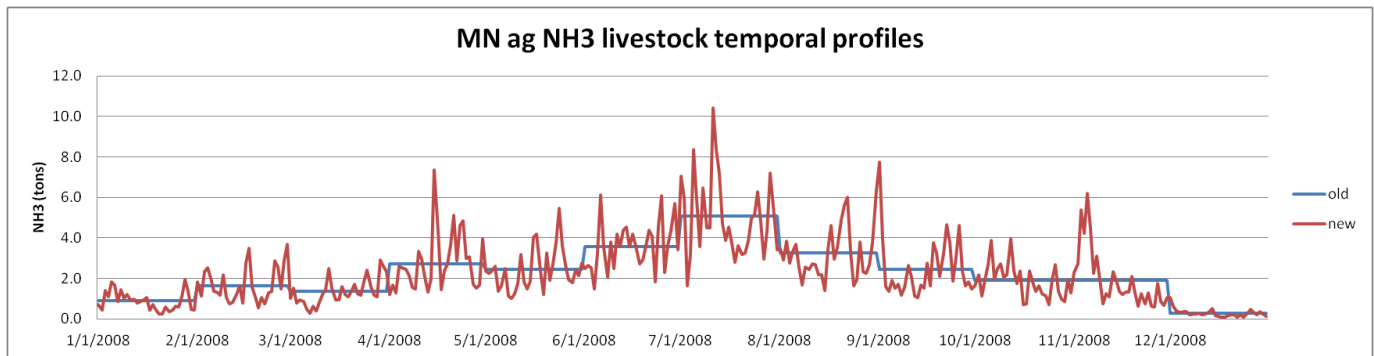

Figure 3--12. Example of animal NH_3 emissions temporalization approaches, summed to daily emissions

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 measurable 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 this 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. RPP uses the gridded minimum and maximum temperature for the day. The combination of these four processes (RPD, RPV, RPH, and RPP) is the total onroad sector emissions. The onroad sector shows a strong meteorological influence on its temporal patterns.

Figure 3-13 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.
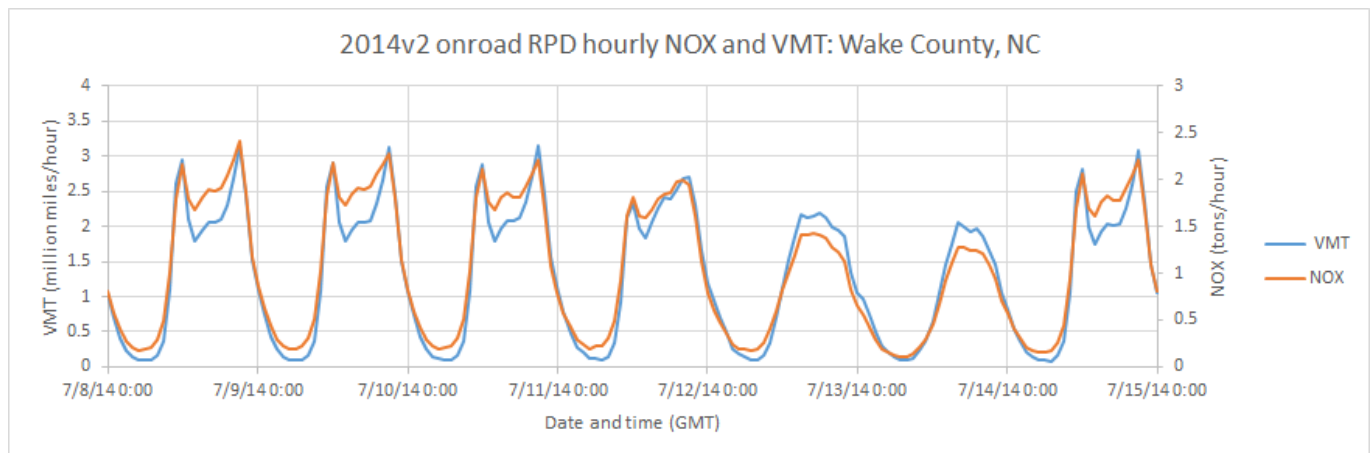
Figure 3-13. Example of SMOKE-MOVES temporal variability of NO$_X$ emissions versus activity

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 data were also temporalized from month to day-of-the-week, and

then to hourly through temporal profiles. The RPD processes use an average speed distribution (SPDIST) that specifies the amount of time spent in each MOVES speed bin for each county, vehicle (aka source) type, road type, weekday/weekend, and hour of day. Unlike other sectors, the temporal profiles and SPDIST 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.

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

The CRC A-100 dataset includes temporal profiles for individual counties, Metropolitan Statistical Areas (MSAs), and entire regions (e.g., West, South). Counties without temporal profiles specific to itself, or to its MSA, are assigned to regional temporal profiles. Temporal profiles also vary between MOVES road types, and there are distinct hour-of-day profiles for each day of the week. Plots of hour-of-day profiles for passenger vehicles in Fulton County, GA, are shown in Figure 3-14. Separate plots are shown for Monday, Friday, Saturday, and Sunday, and each line corresponds to a particular MOVES road type (e.g. road type 2 = rural restricted). Figure 3-15 shows which counties have temporal profiles specific to that county, and which counties use regional average profiles in the CRC A-100 data.
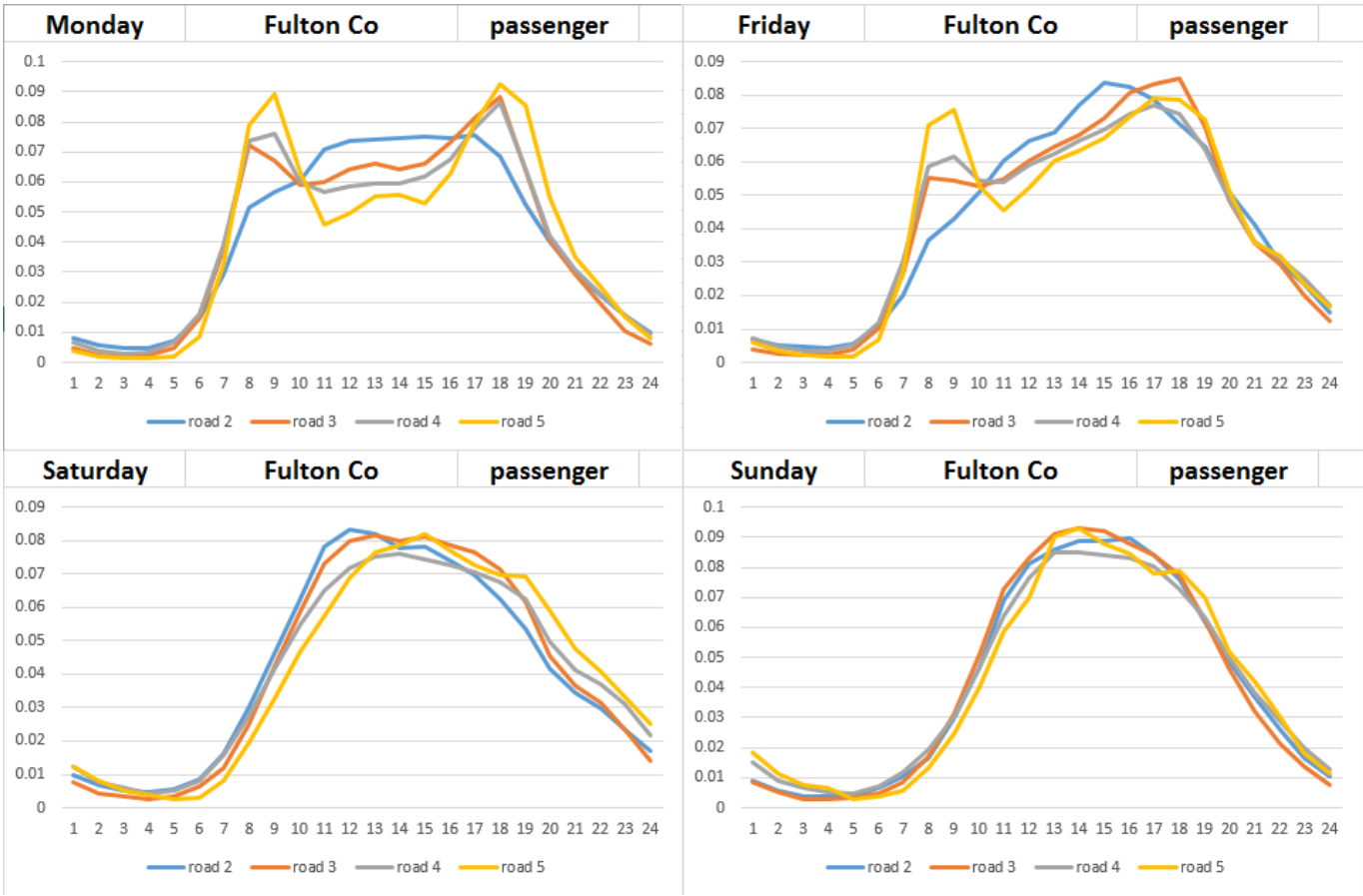
Figure 3-14. Sample onroad diurnal profiles for Fulton County, GA
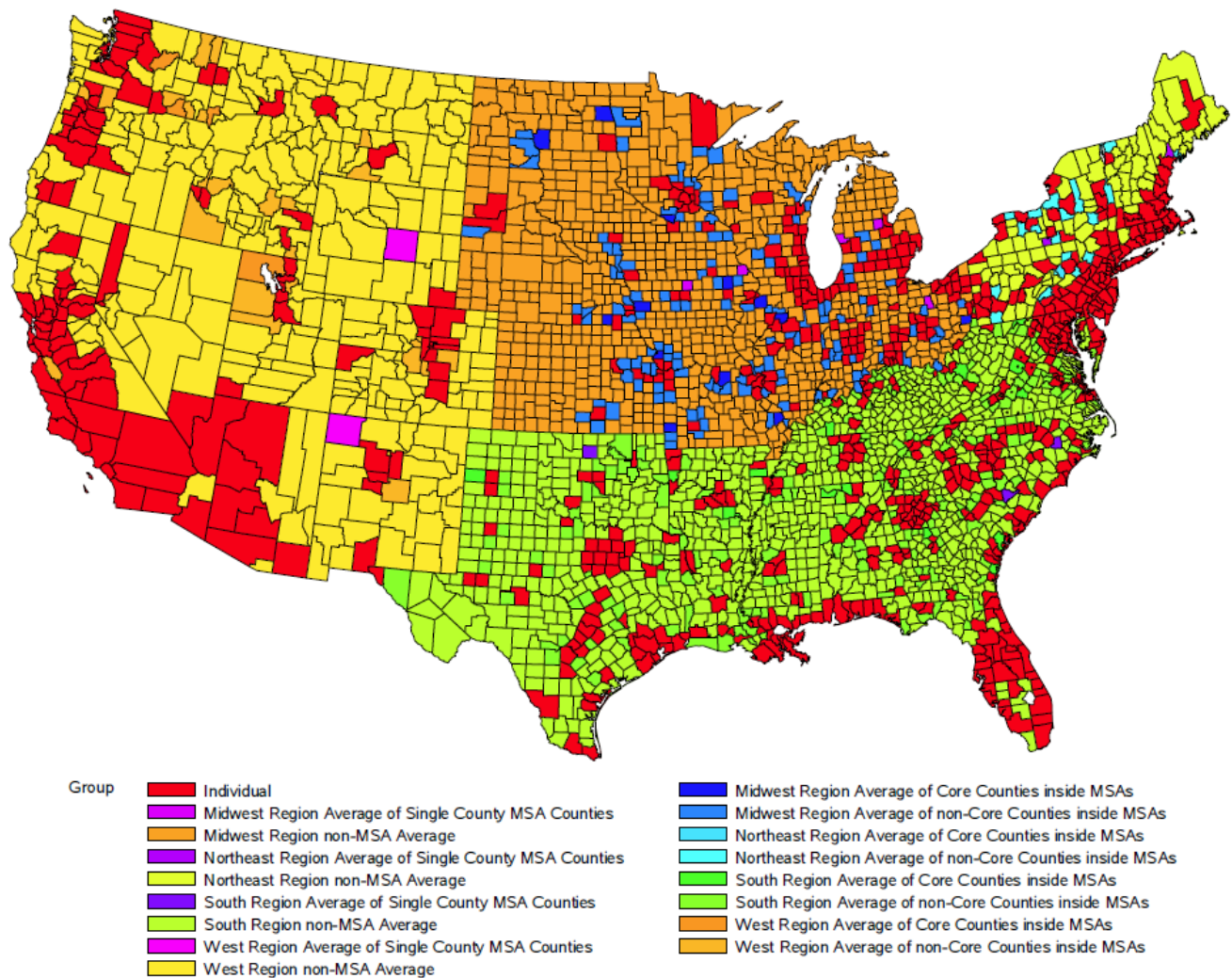
Figure 3-15. Counties for which MOVES Speeds and Temporal Profiles could be Populated

For hoteling, day-of-week profiles are the same as non-hoteling for combination trucks, while hour-of-day non-hoteling profiles for combination trucks were inverted to create new hoteling profiles that peak overnight instead of during the day.

State/local-provided data for the 2017 NEI were accepted for use in the 2017 NEI if they were deemed to be at least as credible as the CRC A-100 data. The 2017 NEI TSD includes more details on which data were used for which counties. In areas of the contiguous United States where state/local-provided data were not provided or deemed unacceptable, the CRC A-100 temporal profiles were used, except in California. All California temporal profiles were carried over from the 2014v7.1 platform, although California hoteling uses CRC A-100-based profiles just like the rest of the country, since CARB didn't have a hoteling-specific profile. Monthly profiles in all states (national profiles by broad vehicle type) were also carried over from 2014v1 and applied directly to the VMT. For California, CARB supplied diurnal profiles that varied by vehicle type, day of the week,[10] and air basin. These CARB-specific

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

profiles were used in developing EPA estimates for California. Although the EPA adjusted the total emissions to match interpolated 2016 levels based on California's submitted inventories for 2014 and 2017, 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 section 3.2.5.1.

3.3.6 *Vertical Allocation of Emissions*

Table 3-7 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, pt_oilgas, ptfire-rx, ptfire-wild, ptagfire, ptfire_othna, 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 traditional stack parameters. However, the ptfire-rx, ptfire-wild, ptagfire, and ptfire_othna inventories do contain data on the acres burned (acres per day) 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. Note that the implementation of fire plume rise in CMAQ differs from the implementation of plume rise in SMOKE 4.8. This study uses CMAQ to compute the fire plume rise.

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 2016-2017 data wherever possible. For Mexico, updated spatial surrogates were used as described below. For Canada, shapefiles for generating new surrogates were provided by ECCC for use with their 2015 inventories. The U.S., Mexican, and Canadian 12-km surrogates cover the entire CONUS domain 12US1 shown in Figure 3-3.

3.3.7.1 Surrogates for U.S. Emissions

There are more than 70 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 this 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.

Some surrogates were updated or newly developed for use in the 2017 platform using recently available data sets, although all 2017 platform surrogates were rerun to ensure they cover an extent consistent with EPA's 36US3 grid. The 2011 National Land Cover Database is used including 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). Onroad surrogates for this platform do not distinguish between urban and rural road types, which prevents issues in areas where there are inconsistent urban and rural definitions between MOVES and the surrogate data.

Surrogate updates made for this 2018 study include:

- A new public school surrogate (508) was developed for off-network school buses

- Corrections were made to the rail surrogates (261/271)

- The transit bus terminal surrogate was re-gapfilled with the NLCD medium+high surrogate (306)

- Some gridding cross reference corrections / updates were made including the use of NLCD medium+high surrogate instead of intercity bus terminals for off network emissions from other buses.

- The 500 series surrogates are no longer used and SCCs that used them (e.g., cigarette smoke, accidental releases) were remapped to NLCD surrogates.

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

Table 3-12. U.S. Surrogates available for the 2018 modeling platform

Code	Surrogate Description	Code	Surrogate Description
N/A	Area-to-point approach (see 3.6.2)	650	Refineries and Tank Farms
100	Population	670	Spud Count - CBM Wells
110	*Housing*	671	Spud Count - Gas Wells
150	Residential Heating - Natural Gas	672	Gas Production at Oil Wells
170	Residential Heating - Distillate Oil	673	*Oil Production at CBM Wells*
180	Residential Heating – Coal	674	Unconventional Well Completion Counts
190	Residential Heating - LP Gas	676	*Well Count - All Producing*
205	Extended Idle Locations	677	*Well Count - All Exploratory*
239	Total Road AADT	678	Completions at Gas Wells
240	Total Road Miles	679	Completions at CBM Wells

Code	Surrogate Description	Code	Surrogate Description
242	All Restricted AADT	681	Spud Count - Oil Wells
244	All Unrestricted AADT	683	Produced Water at All Wells
258	*Intercity Bus Terminals*	6831	Produced Water at CBM Wells
259	Transit Bus Terminals	6832	Produced Water at Gas Wells
260	*Total Railroad Miles*	6833	Produced Water at Oil Wells
261	NTAD Total Railroad Density	685	Completions at Oil Wells
271	NTAD Class 1 2 3 Railroad Density	686	*Completions at All Wells*
300	NLCD Low Intensity Development	687	Feet Drilled at All Wells
304	NLCD Open + Low	691	Well Counts - CBM Wells
305	NLCD Low + Med	692	Spud Count - All Wells
306	NLCD Med + High	693	Well Count - All Wells
307	NLCD All Development	694	Oil Production at Oil Wells
308	NLCD Low + Med + High	695	Well Count - Oil Wells
309	NLCD Open + Low + Med	696	Gas Production at Gas Wells
310	NLCD Total Agriculture	697	Oil Production at Gas Wells
319	NLCD Crop Land	698	Well Count - Gas Wells
320	NLCD Forest Land	699	Gas Production at CBM Wells
321	NLCD Recreational Land	711	Airport Areas
340	*NLCD Land*	801	Port Areas
350	NLCD Water	805	*Offshore Shipping Area*
500	*Commercial Land*	806	*Offshore Shipping NEI2014 Activity*
505	*Industrial Land*	807	*Navigable Waterway Miles*
506	*Education*	808	*2013 Shipping Density*
508	Public Schools	820	*Ports NEI2014 Activity*
510	*Commercial plus Industrial*	850	Golf Courses
535	*Residential + Commercial + Industrial + Institutional + Government*	860	Mines
560	*Hospital (COM6)*		

For the onroad sector, the on-network (RPD) emissions were allocated differently from the off-network (RPP, starts, ONI, and RPV). On-network used average annual daily traffic (AADT) data and off network used land use surrogates as shown in Table 3-13. Emissions from the 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 2016 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	Other Bus	306	NLCD Med + High
42	Transit Bus	259	Transit Bus Terminals
43	School Bus	508	Public Schools

Source type	Source Type name	Surrogate ID	Description
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 2017 data consistent with what was used to develop the 2017 nonpoint oil and gas emissions. The exploration and production of oil and gas has increased in terms of quantities and locations over the last seven years, primarily through the use of new technologies, such as hydraulic fracturing. ERG prepared census-tract, 2-km, and 4-km sub-county surrogate factors for use in 2017 emissions modeling. A technical memo by ERG provides technical details of how the gridding surrogates were generated (ERG, 2019).

Spatial allocation of np_oilgas emissions to the national 36km and 12km domains used for air quality modeling is accomplished using the spatial surrogates described in ERG's technical memo. All spatial surrogates for np_oilgas are developed based on known locations of oil and gas activity for year 2017.

These spatial surrogates, numbered 670 through 699 and also including 6831, 6832, and 6833, were originally processed at 4km resolution and without gapfilling. The surrogates were first gapfilled using fallback surrogates. For each surrogate, the last two fallbacks were surrogate 693 (Well Count – All Wells) and 304 (NLCD Open + Low). Where appropriate, other surrogates were also part of the gapfilling procedure. For example, surrogate 670 (Spud Count – CBM Wells) was first gapfilled with 692 (Spud Count – All Wells), and then 693 and finally 304. After gapfilling, surrogates were aggregated to 12km and 36km resolution. All gapfilling and aggregating was performed with the Surrogate Tool.

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
6831	Produced Water at CBM Wells
6832	Produced Water at Gas Wells
6833	Produced Water at Oil Wells

Surrogate Code	Surrogate Description
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 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 3-15. Selected 2018 CAP emissions by sector for U.S. Surrogates (CONUS domain totals, tons)

Sector	ID	Description	NH$_3$	NO$_X$	PM$_{2.5}$	SO$_2$	VOC
afdust	240	Total Road Miles	0	0	312,090	0	0
afdust	304	NLCD Open + Low	0	0	842,116	0	0
afdust	306	NLCD Med + High	0	0	52,278	0	0
afdust	308	NLCD Low + Med + High	0	0	117,047	0	0
afdust	310	NLCD Total Agriculture	0	0	791,881	0	0
livestock	310	NLCD Total Agriculture	2,571,573	0	0	0	225,550
nonpt	100	Population	34,304	0	0	0	208
nonpt	150	Residential Heating - Natural Gas	33,550	204,371	4,041	1,365	12,055
nonpt	170	Residential Heating - Distillate Oil	1,531	30,031	3,284	11,510	1,039
nonpt	180	Residential Heating - Coal	1	3	1	3	3
nonpt	190	Residential Heating - LP Gas	98	31,061	163	712	1,181
nonpt	239	Total Road AADT	0	22	541	0	297,798
nonpt	240	Total Road Miles	0	0	0	0	0
nonpt	244	All Unrestricted AADT	0	0	0	0	101,255
nonpt	271	NTAD Class 1 2 3 Railroad Density	0	0	0	0	2,203
nonpt	300	NLCD Low Intensity Development	4,823	19,093	94,548	2,882	72,599
nonpt	304	NLCD Open + Low	0	0	0	0	0

Sector	ID	Description	NH₃	NOₓ	PM₂.₅	SO₂	VOC
nonpt	306	NLCD Med + High	23,668	272,514	245,871	131,592	112,049
nonpt	307	NLCD All Development	85	25,798	110,610	8,169	69,262
nonpt	308	NLCD Low + Med + High	884	156,033	15,683	10,076	10,037
nonpt	310	NLCD Total Agriculture	0	0	38	0	0
nonpt	319	NLCD Crop Land	0	0	97	72	299
nonpt	320	NLCD Forest Land	3,953	68	273	0	279
nonpt	650	Refineries and Tank Farms	0	16	0	0	106,401
nonpt	711	Airport Areas	0	0	0	0	596
nonpt	801	Port Areas	0	0	0	0	6,730
nonroad	261	NTAD Total Railroad Density	3	1,914	198	1	376
nonroad	304	NLCD Open + Low	4	1,690	144	4	2,488
nonroad	305	NLCD Low + Med	95	14,943	3,859	104	106,139
nonroad	306	NLCD Med + High	326	166,683	10,458	297	89,752
nonroad	307	NLCD All Development	101	29,905	15,389	97	170,454
nonroad	308	NLCD Low + Med + High	551	286,527	23,894	234	47,904
nonroad	309	NLCD Open + Low + Med	121	21,137	1,246	135	45,692
nonroad	310	NLCD Total Agriculture	420	329,678	23,876	187	34,856
nonroad	320	NLCD Forest Land	15	3,954	558	8	3,731
nonroad	321	NLCD Recreational Land	83	12,636	5,805	76	215,471
nonroad	350	NLCD Water	191	114,414	4,918	212	293,014
nonroad	850	Golf Courses	13	2,066	118	14	5,685
nonroad	860	Mines	2	2,523	251	1	476
np_oilgas	670	Spud Count - CBM Wells	0	0	0	0	180
np_oilgas	671	Spud Count - Gas Wells	0	0	0	0	5,317
np_oilgas	672	Gas Production at Oil Wells	0	600	0	253	69,913
np_oilgas	674	Unconventional Well Completion Counts	3	21,725	530	259	2,325
np_oilgas	678	Completions at Gas Wells	0	9,654	236	3,577	21,788
np_oilgas	679	Completions at CBM Wells	0	3	0	98	607
np_oilgas	681	Spud Count - Oil Wells	0	0	0	0	32,076
np_oilgas	683	Produced Water at All Wells	0	24	0	0	940
np_oilgas	685	Completions at Oil Wells	0	1,007	0	483	46,741
np_oilgas	687	Feet Drilled at All Wells	5	43,220	1,346	225	3,996
np_oilgas	691	Well Counts - CBM Wells	0	19,926	289	7	15,937
np_oilgas	692	Spud Count - All Wells	0	395	13	46	37
np_oilgas	693	Well Count - All Wells	0	0	0	0	2
np_oilgas	694	Oil Production at Oil Wells	0	4,942	0	7,417	991,056
np_oilgas	695	Well Count - Oil Wells	0	157,530	3,832	25,330	529,262
np_oilgas	696	Gas Production at Gas Wells	0	47,302	300	5,805	301,077
np_oilgas	697	Oil Production at Gas Wells	0	930	0	0	87,563
np_oilgas	698	Well Count - Gas Wells	6	357,689	4,846	156	557,838
np_oilgas	699	Gas Production at CBM Wells	0	33	5	0	6,090
np_oilgas	6831	Produced water at CBM wells	0	0	0	0	846

Sector	ID	Description	NH₃	NOₓ	PM₂.₅	SO₂	VOC
np_oilgas	6832	Produced water at gas wells	0	0	0	0	17,872
np_oilgas	6833	Produced water at oil wells	0	0	0	0	92,231
onroad	205	Extended Idle Locations	333	31,740	616	17	3,337
onroad	242	All Restricted AADT	34,519	922,998	23,496	6,667	137,657
onroad	244	All Unrestricted AADT	63,741	1,538,528	53,194	14,424	387,798
onroad	259	Transit Bus Terminals	15	2,725	63	2	510
onroad	304	NLCD Open + Low	0	872	27	0	6,880
onroad	306	NLCD Med + High	927	94,894	3,461	86	19,921
onroad	307	NLCD All Development	3,494	211,798	6,822	1,352	584,337
onroad	308	NLCD Low + Med + High	206	21,756	549	78	31,605
onroad	508	Public Schools	15	2,140	85	1	562
rail	261	NTAD Total Railroad Density	15	35,364	988	32	1,704
rail	271	NTAD Class 1 2 3 Railroad Density	350	535,605	14,016	695	23,244
rwc	300	NLCD Low Intensity Development	16,413	34,093	299,278	7,988	323,969

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" (ARTOPNT) 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://www.epa.gov/sites/production/files/2020-10/documents/emissions_tsd_vol1_02-28-08.pdf.

3.3.7.3   *Surrogates for Canada and Mexico Emission Inventories*

The surrogates for Canada to spatially allocate the Canadian emissions are based on the 2016 Canadian inventories and associated data. The spatial surrogate data came from ECCC, 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. The population surrogate was updated for Mexico for the 2014v7.1 platform. Surrogate code 11, which uses 2015 population data at 1 km resolution, replaces the previous population surrogate code 10. The other surrogates for Mexico are circa 1999 and 2000 and were based on data obtained from the Sistema Municpal de Bases de Datos (SIMBAD) de INEGI and the Bases de datos del Censo Economico 1999. Most of the CAPs allocated to the Mexico and Canada surrogates are shown in Table 3-17. 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	921	Commercial Fuel Combustion
101	total dwelling	923	TOTAL INSTITUTIONAL AND GOVERNEMNT
104	capped total dwelling	924	Primary Industry

Code	Canadian Surrogate Description	Code	Description
106	ALL_INDUST	925	Manufacturing and Assembly
113	Forestry and logging	926	Distribtution and Retail (no petroleum)
200	Urban Primary Road Miles	927	Commercial Services
210	Rural Primary Road Miles	932	CANRAIL
211	Oil and Gas Extraction	940	PAVED ROADS NEW
212	Mining except oil and gas	946	Construction and mining
220	Urban Secondary Road Miles	948	Forest
221	Total Mining	951	Wood Consumption Percentage
222	Utilities	955	UNPAVED_ROADS_AND_TRAILS
230	Rural Secondary Road Miles	960	TOTBEEF
233	Total Land Development	970	TOTPOUL
240	capped population	980	TOTSWIN
308	Food manufacturing	990	TOTFERT
321	Wood product manufacturing	996	urban_area
323	Printing and related support activities	1251	OFFR_TOTFERT
324	Petroleum and coal products manufacturing	1252	OFFR_MINES
326	Plastics and rubber products manufacturing	1253	OFFR Other Construction not Urban
327	Non-metallic mineral product manufacturing	1254	OFFR Commercial Services
331	Primary Metal Manufacturing	1255	OFFR Oil Sands Mines
350	Water	1256	OFFR Wood industries CANVEC
412	Petroleum product wholesaler-distributors	1257	OFFR UNPAVED ROADS RURAL
448	clothing and clothing accessories stores	1258	OFFR_Utilities
482	Rail transportation	1259	OFFR total dwelling
562	Waste management and remediation services	1260	OFFR_water
901	AIRPORT	1261	OFFR_ALL_INDUST
902	Military LTO	1262	OFFR Oil and Gas Extraction
903	Commercial LTO	1263	OFFR_ALLROADS
904	General Aviation LTO	1265	OFFR_CANRAIL
945	Commercial Marine Vessels	9450	Commercial Marine Vessel Ports

Table 3-17. 2018 CAPs Allocated to Mexican and Canadian Spatial Surrogates for 12US1 (tons)

Code	Mexican or Canadian Surrogate Description	NH₃	NOₓ	PM₂.₅	SO₂	VOC
11	MEX 2015 Population	0	83,967	479	173	227,018
14	MEX Residential Heating - Wood	0	2,421	6,789	202	18,159
16	MEX Residential Heating - Distillate Oil	1	29	0	0	1

Code	Mexican or Canadian Surrogate Description	NH₃	NOₓ	PM₂.₅	SO₂	VOC
22	MEX Total Road Miles	2,918	361,090	12,212	6,459	71,786
24	MEX Total Railroads Miles	0	23,678	529	208	919
26	MEX Total Agriculture	111,604	22,061	16,776	532	4,408
32	MEX Commercial Land	0	78	1,701	0	28,740
34	MEX Industrial Land	87	2,219	1,315	6	36,092
36	MEX Commercial plus Industrial Land	4	7,408	373	14	104,786
40	MEX Residential (RES1-4)+Comercial+Industrial+Institutional+Government	0	17	76	2	21,780
42	MEX Personal Repair (COM3)	0	0	0	0	5,311
44	MEX Airports Area	0	4,148	62	271	1,626
48	MEX Brick Kilns	0	276	5,523	500	134
50	MEX Mobile sources - Border Crossing	3	71	2	0	57
100	CAN Population	776	51	604	14	219
101	CAN total dwelling	0	0	0	0	147,322
104	CAN capped total dwelling	347	30,961	2,282	2,473	1,614
106	CAN ALL_INDUST			583		
113	CAN Forestry and logging	117	1,392	7,471	29	3,938
200	CAN Urban Primary Road Miles	1,579	67,175	2,165	315	7,245
210	CAN Rural Primary Road Miles	630	38,422	1,167	130	3,034
211	CAN Oil and Gas Extraction	1	39	424	41	1,657
212	CAN Mining except oil and gas	0	0	3,051	0	0
220	CAN Urban Secondary Road Miles	2,963	106,714	4,346	664	19,264
221	CAN Total Mining	0	0	13,221	0	0
222	CAN Utilities	55	3,344	2,859	453	63
230	CAN Rural Secondary Road Miles	1,659	72,070	2,278	349	8,384
240	CAN capped population	329	47,281	1,340	74	96,299
308	CAN Food manufacturing	0	0	18,982	0	17,387
321	CAN Wood product manufacturing	785	4,450	1,543	328	15,455
323	CAN Printing and related support activities	0	0	0	0	11,693
324	CAN Petroleum and coal products manufacturing	0	1,179	1,599	462	9,154
326	CAN Plastics and rubber products manufacturing	0	0	0	0	24,027
327	CAN Non-metallic mineral product manufacturing	0	0	6,449	0	0
331	CAN Primary Metal Manufacturing	0	156	5,561	29	72
412	CAN Petroleum product wholesaler-distributors	0	0	0	0	43,724

Code	Mexican or Canadian Surrogate Description	NH₃	NOₓ	PM₂.₅	SO₂	VOC
448	CAN clothing and clothing accessories stores	0	0	0	0	140
482	CAN Rail transportation	1	4,062	88	1	256
562	CAN Waste management and remediation services	240	1,924	2,620	2,483	9,199
901	CAN AIRPORT	0	93	9	0	9
921	CAN Commercial Fuel Combustion	187	24,020	2,379	1,414	1,224
923	CAN TOTAL INSTITUTIONAL AND GOVERNEMNT	0	0	0	0	14,458
924	CAN Primary Industry	0	0	0	0	38,858
925	CAN Manufacturing and Assembly	0	0	0	0	69,488
926	CAN Distribtution and Retail (no petroleum)	0	0	0	0	7,285
927	CAN Commercial Services	0	0	0	0	31,311
932	CAN CANRAIL	48	83,844	1,662	43	3,559
940	CAN PAVED ROADS NEW			27,751		
946	CAN Construction and mining	0	0	0	0	9,850
951	CAN Wood Consumption Percentage	957	10,634	107,554	1,519	152,072
955	CAN UNPAVED_ROADS_AND_TRAILS			383,147		
990	CAN TOTFERT	48	4,047	265	6,827	152
996	CAN urban_area	0	0	2,994	0	0
1251	CAN OFFR_TOTFERT	73	54,477	3,738	49	5,024
1252	CAN OFFR_MINES	1	576	39	1	84
1253	CAN OFFR Other Construction not Urban	66	31,684	3,880	41	10,454
1254	CAN OFFR Commercial Services	42	14,790	2,278	33	35,408
1255	OFFR Oil Sands Mines	0	0	0	0	0
1256	CAN OFFR Wood industries CANVEC	7	2,292	223	4	875
1257	CAN OFFR UNPAVED ROADS RURAL	24	10,294	603	18	25,750
1258	CAN OFFR_Utilities	8	3,857	187	6	838
1259	CAN OFFR total dwelling	17	5,963	600	13	12,541
1260	CAN OFFR_water	19	5,544	307	26	22,607
1261	CAN OFFR_ALL_INDUST	4	5,187	154	2	1,064
1262	CAN OFFR Oil and Gas Extraction	1	580	41	0	164
1263	CAN OFFR_ALLROADS	3	1,480	143	2	447
1265	CAN OFFR_CANRAIL	0	493	16	0	38

3.4   Emissions References

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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 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.[11] 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 2018 assessment used a single domain that covers the entire continental U.S. (CONUS) and large portions of Canada and Mexico using 12-km by 12-km horizontal grid spacing. Currently, 12-km x 12-km resolution is sufficient

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[11] 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.

as the highest resolution for most regional-scale air quality model applications and assessments.[12] 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 include 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.[13]

4.2   CMAQ Model Version, Inputs and Configuration

This section describes the air quality modeling platform used for the 2018 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 the region modeled. We used the CMAQ modeling system as part of the 2018 Platform to provide a national

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[12] U.S. EPA (2018), Modeling Guidance for Demonstrating Air Quality Goals for Ozone, PM2.5, and Regional Haze, pp 205. https://www3.epa.gov/ttn/scram/guidance/guide/O3-PM-RH-Modeling_Guidance-2018.pdf.
[13] 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.

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 PM$_{2.5}$.

This section provides a description of each of the main components of the 2018 CMAQ simulation along with the results of a model performance evaluation in which the 2018 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 particle pollutants in the atmosphere. This 2018 analysis employed CMAQ version 5.3.2.[14] The 2018 CMAQ run included CB6r3 chemical mechanism, AERO7 aerosol module with non-volatile Primary Organic Aerosol (POA). The CMAQ community model versions 5.0.2 and 5.1 were most recently peer-reviewed in September of 2016 for the U.S. EPA.[15]

4.2.2 Model Domain and Grid Resolution

The 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 2018 simulation used a Lambert Conformal map projection centered at (-97, 40) with true latitudes at 33 and 45 degrees north. The 12-km 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 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 2018 simulation. Air quality conditions at the outer boundary of the 12-km domain were taken from the northern hemispheric CMAQ model (discussed in Section 4.2.4).

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[14] CMAQ version 5.3.2: https://doi.org/10.5281/zenodo.4081737; https://www.epa.gov/cmaq/cmaq-models-0. CMAQ v5.3.2 is also available from the Community Modeling and Analysis System (CMAS) at: http://www.cmascenter.org.

[15] 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 2018 12-km Modeling Domain

National 12 km 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 2018 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
12	0.9100	914.50	714
11	0.9200	924.00	632
10	0.9300	933.50	551
9	0.9400	943.00	470

Vertical Layers	Sigma P	Pressure (mb)	Approximate Height (m)
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

12km CONUS nationwide domain
x,y: -2556000,-1728000
col: 459 row: 299
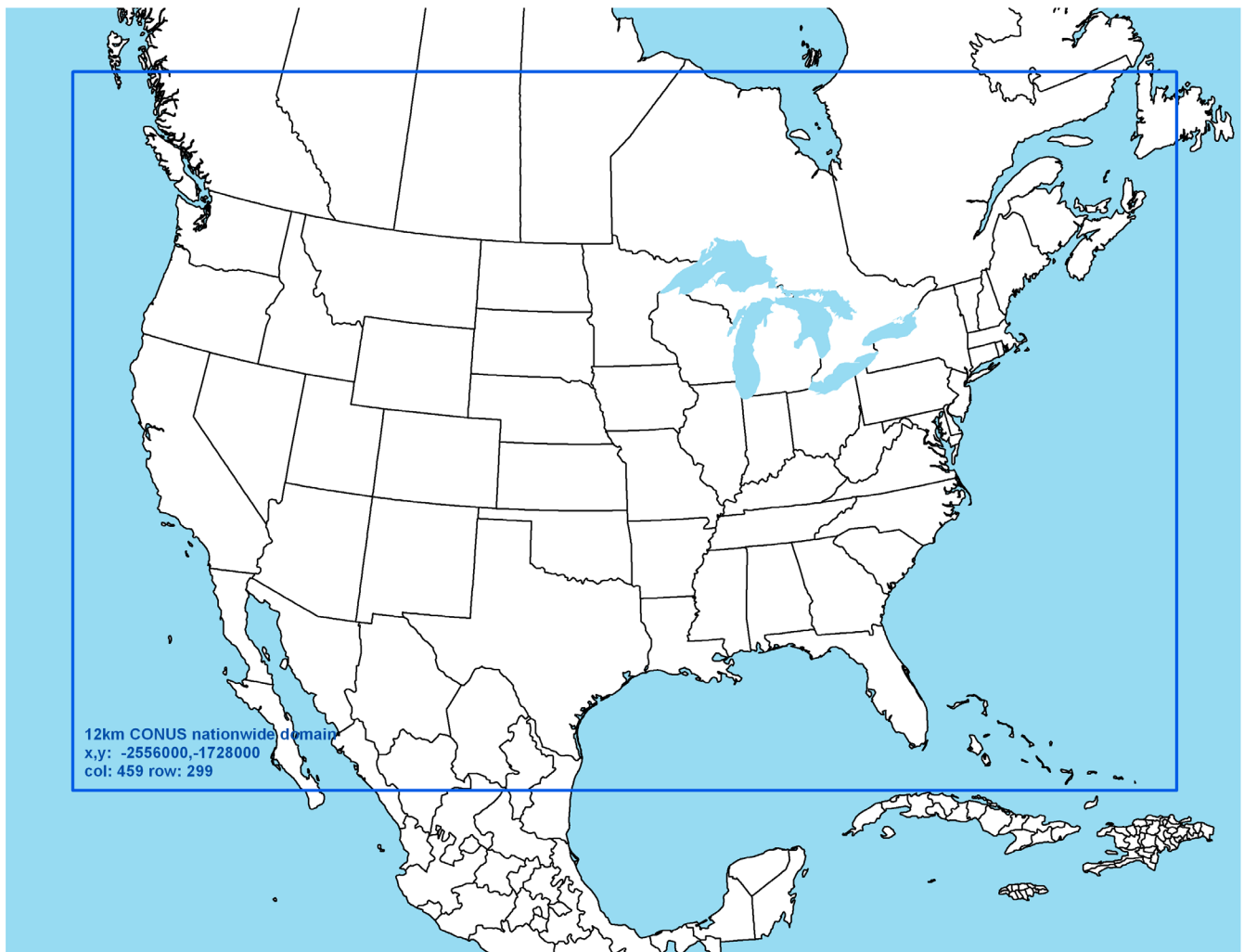
Figure 4-1. Map of the 2018 CMAQ Modeling Domain. The blue box denotes the 12-km national modeling domain.

4.2.3 Modeling Period / Ozone Episodes

The 12-km CMAQ modeling domain was modeled for the entire year of 2018. The annual simulation included a spin-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

2018 Emissions: The emissions inventories used in the 2018 air quality modeling are described in Section 3, above.

2018 Meteorological Input Data: The gridded meteorological data for the entire year of 2018 at the 12-km continental United States scale domain was derived from the publicly available version 3.8 of the Weather Research and Forecasting Model (WRF), Advanced Research WRF (ARW) core.[16] 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 12US WRF model was initialized using the 12-km North American Model (12NAM)[17] analysis product provided by National Climatic Data Center (NCDC). Where 12NAM data was unavailable, the 40-km Eta Data Assimilation System (EDAS) analysis (ds609.2) from the National Center for Atmospheric Research (NCAR) was used. Analysis nudging for temperature, wind, and moisture was applied above the boundary layer only. The model simulations were conducted continuously. The 'ipxwrf' program was used to initialize deep soil moisture at the start of the run using a 10-day spin-up period. The 2018 WRF meteorology simulated was based on 2011 National Land Cover Database (NLCD).[18] The WRF simulation included the physics options of the Pleim-Xiu land surface model (LSM), Asymmetric Convective Model version 2 planetary boundary layer (PBL) scheme, Morrison double moment microphysics, Kain- Fritsch cumulus parameterization scheme utilizing the moisture-advection trigger[19] and the RRTMG long-wave and shortwave radiation (LWR/SWR) scheme.[20] These simulations also incorporated observed lightning data from the National Lightning Detection Network (NLDN) to suppress (force) deep convection where lightning is absent (present).[21] In addition, the Group for High Resolution

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[16] 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.

[17] North American Model Analysis-Only, http://nomads.ncdc.noaa.gov/data.php; download from ftp://nomads.ncdc.noaa.gov/NAM/analysis_only/.

[18] National Land Cover Database 2011, http://www.mrlc.gov/nlcd2011.php.

[19] 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.

[20] 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.

[21] Heath, Nicholas K., Pleim, J.E., Gilliam, R., Kang, D., 2016. A simple lightning assimilation technique for improving retrospective WRF simulations. Journal of Advances in Modeling Earth Systems. 8. 10.1002/2016MS000735.

Sea Surface Temperatures (GHRSST)[22,23] 1-km SST data was used for SST information to provide more resolved information compared to the more coarse data in the NAM analysis.

2018 Initial and Boundary Conditions: The lateral boundary and initial species concentrations were provided by a global application of GEOS-Chem [24] to the year 2018. The global-scale platform uses v12.0.1 (doi: 10.5281/zenodo.1403144) at 2 x 2.5-degree resolution (half cells at the north and south pole) with year-specific meteorology for 2018. Meteorology is provided by the Goddard Earth Observation System Forward Product (GEOS_FP) using 72 vertical layers from the surface to 0.01 hPa. The GEOS-Chem standard chemistry option was applied at all levels. Emissions were provided using the standard configuration of the Harmonized Emissions Component (HEMCO)[25] distributed with v12.0.1 of GEOS-Chem. The biogenic, soil NOx, dust, and sea salt emissions were all calculated online using the GEOS-FP 2018 emissions. At the time this simulation was run, GEOS-Chem did not have updated fire emissions for 2018. For this run, 2016 monthly fire emissions were used as a climatology. Note this would have larger implications for applying the model over the continental US, but less so for lateral boundary conditions. The anthropogenic configuration uses a combination of the Community Emissions Data System (CEDS)[26] from the 2014 year with regional inventories superseding CEDS. For example, regional inventories are used over the United States, Mexico, Canada, and Europe. These inventories have differing base years and are projected to a nominal present day using either International Energy Agency fuel statistics or using regional emission trends.

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 2018 simulation using state/local monitoring sites data in order to estimate the ability of the CMAQ modeling system to replicate the 2018 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.

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[22] 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.

[23] Global High-Resolution SST (GHRSST) analysis, https://www.ghrsst.org/.

[24] Bey, I., D. J. Jacob, R. M. Yantosca, J. A. Logan, B. Field, A. M. Fiore, Q. Li, H. Liu, L. J. Mickley, and M. Schultz, Global modeling of tropospheric chemistry with assimilated meteorology: Model description and evaluation, J. Geophys. Res., 106, 23,073-23,096, doi:10.1029/2001JD000807, 2001.

[25] Keller, C.A., M.S. Long, R.M. Yantosca, A.M. Da Silva, S. Pawson, and D.J. Jacob, HEMCO v1.0: A versatile, ESMF-compliant component for calculating emissions in atmospheric models, Geosci. Model Devel., 7, 1409-1417, doi:10.5194/gmd-7-1409-2014, 2014.

[26] Hoesly, R. M., Smith, S. J., Feng, L., Klimont, Z., Janssens-Maenhout, G., Pitkanen, T., Seibert, J. J., Vu, L., Andres, R. J., Bolt, R. M., Bond, T. C., Dawidowski, L., Kholod, N., Kurokawa, J.-I., Li, M., Liu, L., Lu, Z., Moura, M. C. P., O'Rourke, P. R., and Zhang, Q.: Historical (17502014) anthropogenic emissions of reactive gases and aerosols from the Community Emissions Data System (CEDS), Geosci. Model Dev., 11, 369-408, doi: 10.5194/gmd-11-369-2018, 2018.

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:

$$MB = \frac{1}{n}\sum_1^n (P - O) \text{ , where P = predicted and O = observed concentrations.}$$

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:

$$ME = \frac{1}{n}\sum_1^n |P - O|$$

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:

$$NMB = \frac{\sum_1^n (P - O)}{\sum_1^n (O)} *100 \text{, where P = predicted concentrations and O = observed}$$

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

$$NME = \frac{\sum_1^n |P - O|}{\sum_1^n (O)} *100$$

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[27] 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[28,29] as were originally identified in Karl and Koss (1984).[30]

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[27] 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.

[28] 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.

[29] 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.

[30] 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.
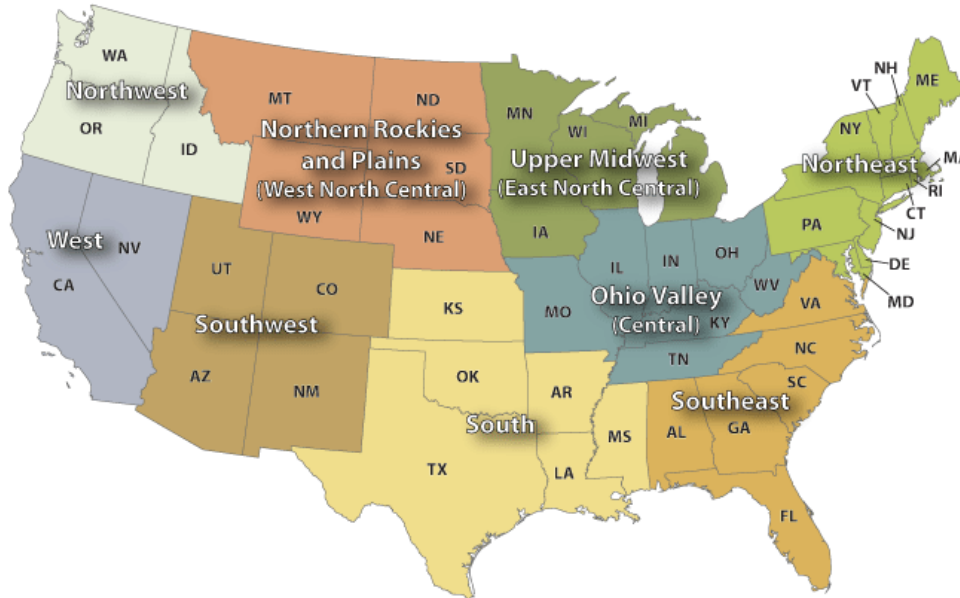
Figure 4-2. NOAA Nine Climate Regions (source: http://www.ncdc.noaa.gov/monitoring-references/maps/us-climate-regions.php#references)

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 in the continental U.S. were included in the evaluation and were taken from the 2018 state/local monitoring site data in 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 2018 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 and CASTNet sites in the summer is over predicted at all climate regions (NMB ranging between 0.1 to 10.5 percent) except in the Northern Rockies, Northwest, West and in the Upper Midwest at CASTNet sites only where there is a slight under prediction. Likewise, 8-hour ozone at the AQS

and CASTNet sites in the winter is over predicted across the contiguous U.S. (NMB ranging between 3.8 to 15.4 percent). In the fall, 8-hour ozone is typically over predicted (bias ranges from 2.4% to 17.7%) except at the Southwest CASTNet sites and in the West and AQS and CASTNet sites. However, 8-hour ozone concentrations in the spring are under predicted at AQS and CASTNet sites in all of the NOAA climate regions (with NMBs less than approximately 20 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 4-3 shows the mean bias for 8-hour daily maximum ozone greater than 60 ppb is generally ±15 ppb across the AQS and CASTNet sites. Likewise, the information in Figure 4-5 indicates that the normalized mean 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 16 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, Upper Midwest, Southeast, along portions of the Gulf Coast, and Great Lakes coastline.

Table 4-4. Summary of CMAQ 2018 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	10,990	2.8	4.6	8.9	14.4
		Spring	16,222	-3.0	5.9	-6.6	12.9
		Summer	16,416	0.9	5.9	2.0	13.6
		Fall	13,174	5.3	6.3	17.7	21.2
	CASTNet	Winter	1,259	2.1	3.9	6.1	11.3
		Spring	1,317	-4.1	6.1	-8.7	12.9
		Summer	1,345	0.5	5.8	1.2	14.1
		Fall	1,310	4.9	5.8	16.3	19.1
Ohio Valley	AQS	Winter	7,466	4.5	5.7	15.4	19.8
		Spring	20,991	-2.0	5.4	-4.4	11.6
		Summer	21,020	1.3	5.7	2.9	12.4
		Fall	16,044	4.7	6.2	14.9	19.6
	CASTNet	Winter	1,542	3.0	4.9	9.3	15.3
		Spring	1,581	-3.3	5.7	-6.8	12.0
		Summer	1,586	1.2	5.3	2.7	12.2
		Fall	1,587	3.8	5.7	11.9	17.9
Upper Midwest	AQS	Winter	2,287	4.3	5.3	13.4	16.5
		Spring	8,951	-3.1	5.7	-6.6	12.0
		Summer	8,913	0.0	5.3	0.1	12.6

Climate region	Monitor Network	Season	No. of Obs	MB (ppb)	ME (ppb)	NMB (%)	NME (%)
		Fall	6,347	0.6	4.8	15.9	20.4
	CASTNet	Winter	442	3.0	4.2	8.7	12.3
		Spring	452	-6.2	6.9	-12.5	13.8
		Summer	447	-2.7	5.4	-6.4	13.2
		Fall	441	4.4	5.2	14.7	17.4
	AQS	Winter	7,020	0.9	3.8	2.5	10.9
		Spring	15,659	-2.6	6.0	-5.7	13.2
		Summer	15,099	4.1	6.8	10.5	17.3
		Fall	11,481	3.2	5.1	9.5	15.3
Southeast							
	CASTNet	Winter	869	0.6	3.9	1.8	11.0
		Spring	926	-4.3	6.5	-9.0	13.8
		Summer	885	2.2	6.0	5.6	15.2
		Fall	812	3.0	5.2	8.9	15.5
	AQS	Winter	10,905	2.2	5.1	7.2	16.7
		Spring	13,080	-2.7	6.4	-5.8	13.5
		Summer	12,839	2.9	7.4	7.0	17.8
		Fall	12,228	3.2	6.2	10.1	19.3
South							
	CASTNet	Winter	514	2.0	4.8	5.9	14.5
		Spring	548	-3.7	6.4	-7.7	13.4
		Summer	508	0.6	6.9	1.5	16.1
		Fall	486	3.6	5.7	11.2	17.6
	AQS	Winter	9,867	1.8	5.0	4.7	13.1
		Spring	10,979	-5.2	6.4	-9.7	11.9
		Summer	11,181	-2.9	6.6	-5.0	11.3
		Fall	10,779	1.0	4.8	2.4	11.7
Southwest							
	CASTNet	Winter	749	0.0	3.3	-0.1	7.5
		Spring	783	-5.6	6.4	-10.3	11.7
		Summer	789	-1.8	5.3	-3.2	9.2
		Fall	778	-0.2	3.9	-0.5	8.7
	AQS	Winter	4,602	3.1	4.6	8.4	12.4
Northern Rockies		Spring	4,992	-2.6	5.9	-5.5	12.3
		Summer	5,031	-2.0	6.1	-4.2	12.9
		Fall	4,894	3.0	5.4	8.5	15.5

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Climate region	Monitor Network	Season	No. of Obs	MB (ppb)	ME (ppb)	NMB (%)	NME (%)
	CASTNet	Winter	513	2.2	4.4	5.3	10.8
		Spring	529	-4.8	5.4	-9.5	11.7
		Summer	509	-3.2	5.5	-6.2	10.5
		Fall	436	1.1	4.3	2.7	10.4
Northwest	AQS	Winter	664	1.9	5.1	6.0	15.9
		Spring	1,426	-1.6	5.9	-4.0	14.8
		Summer	2,400	-0.4	6.1	-1.1	14.9
		Fall	1,137	1.9	5.4	5.5	16.1
	CASTNet	Winter	79	2.3	4.8	6.5	13.8
		Spring	91	-4.6	5.5	-10.5	12.6
		Summer	90	-5.4	6.8	-11.7	14.9
		Fall	90	1.4	5.7	4.2	16.8
West	AQS	Winter	13,866	1.3	5.7	3.8	16.7
		Spring	16,826	-4.7	6.3	-10.1	13.5
		Summer	17,444	-3.6	8.2	-6.7	15.4
		Fall	16,084	-2.8	6.5	-6.3	14.5
	CASTNet	Winter	515	1.8	5.3	4.4	13.2
		Spring	540	-5.9	6.7	-11.8	13.4
		Summer	528	-7.6	10.0	-12.2	16.0
		Fall	523	-3.7	6.4	-7.5	13.0
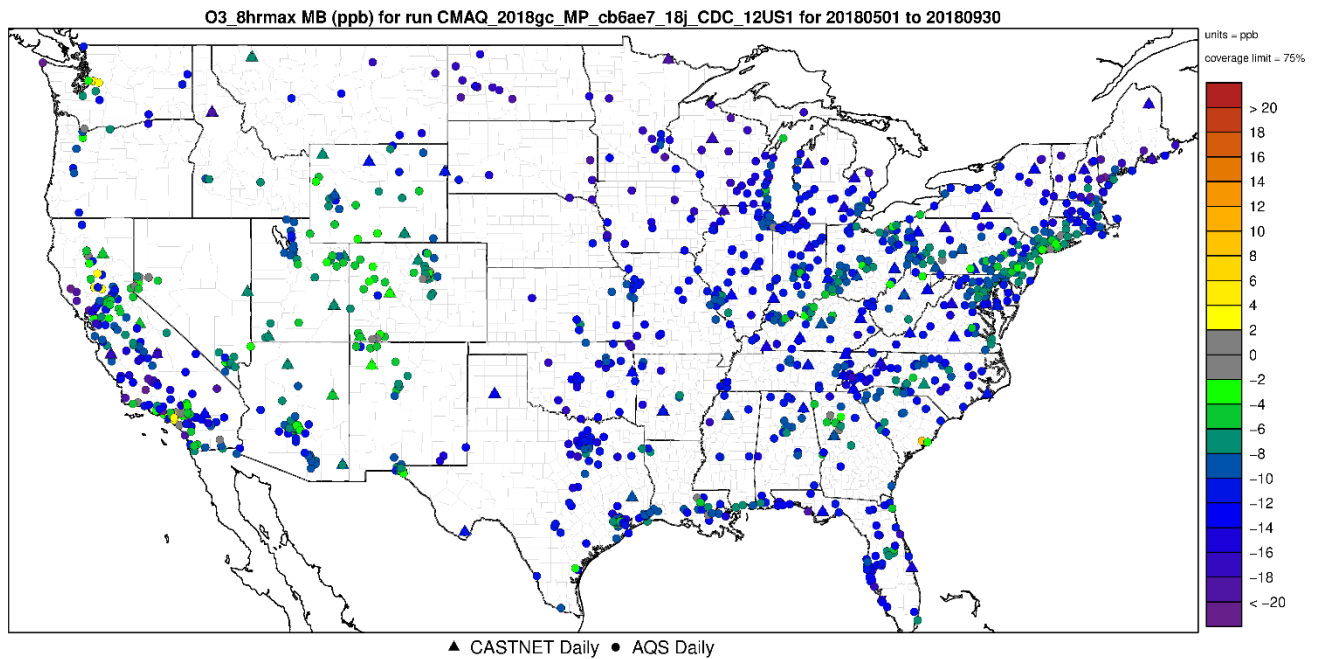
Figure 4-3. Mean Bias (ppb) of 8-hour daily maximum ozone greater than 60 ppb over the period May-September 2018 at AQS and CASTNet monitoring sites in the continental U.S. modeling domain.
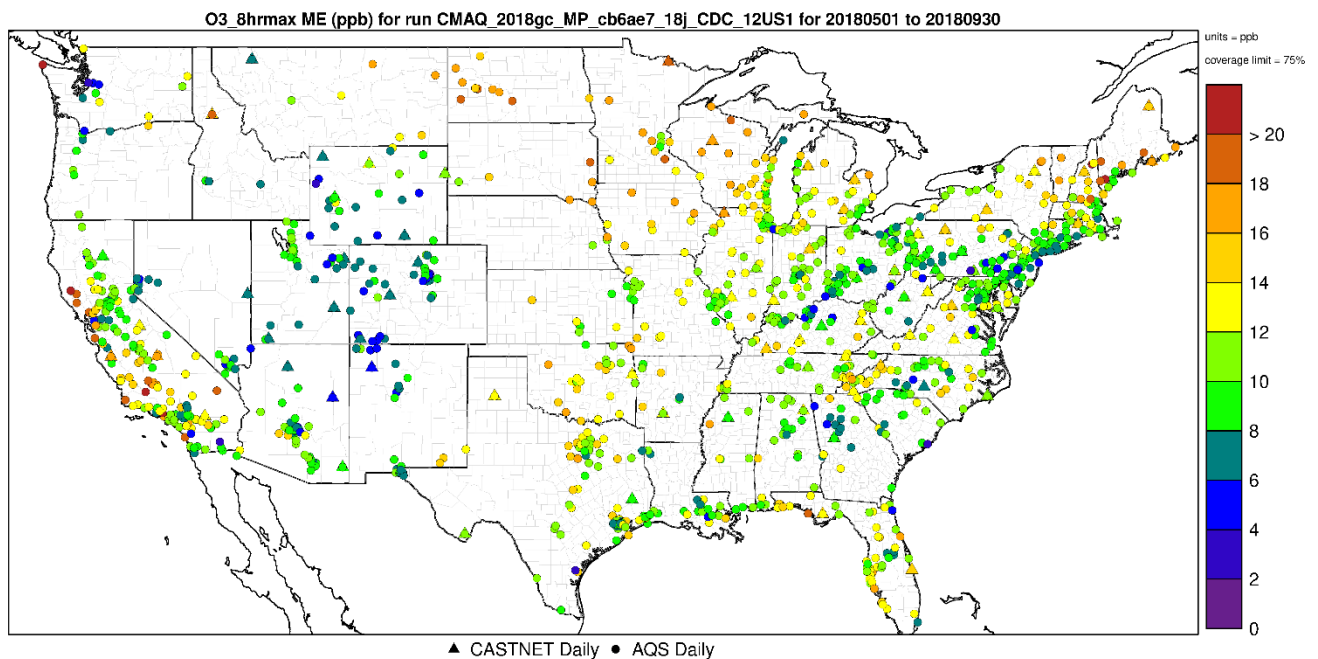
Figure 4-4. Mean Error (ppb) of 8-hour daily maximum ozone greater than 60 ppb over the period May-September 2018 at AQS and CASTNet monitoring sites in the continental U.S. modeling domain.
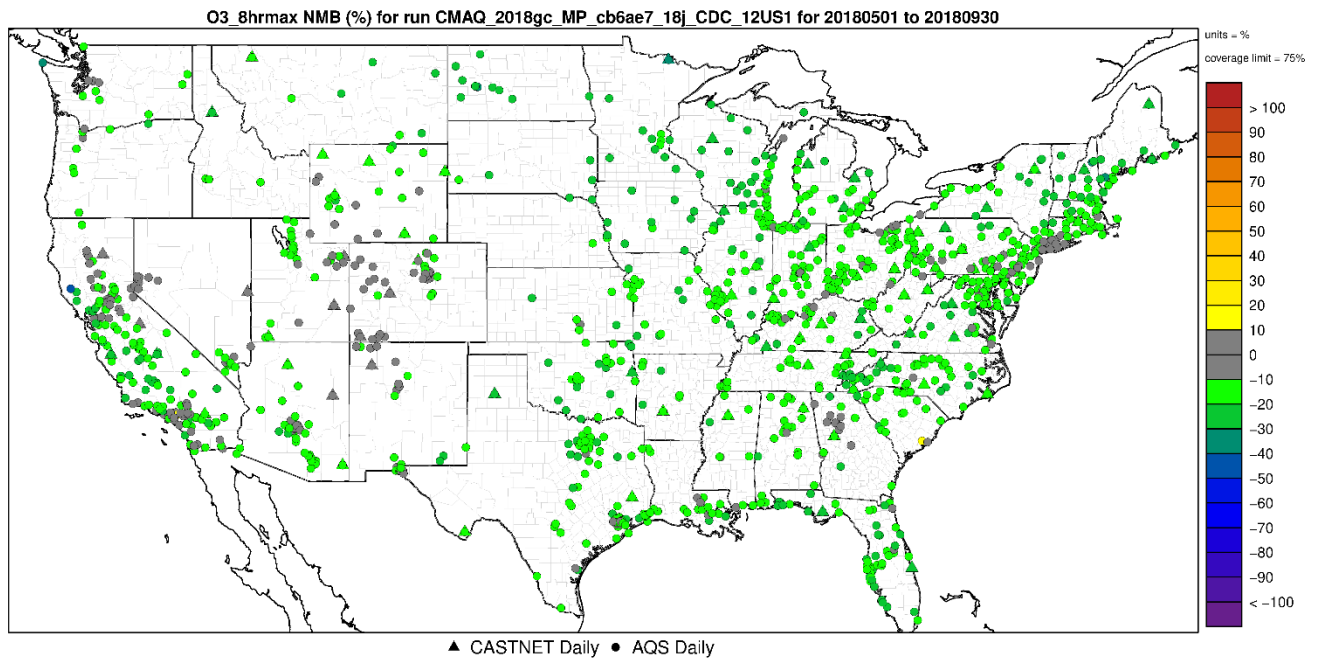
Figure 4-5. Normalized Mean Bias (%) of 8-hour daily maximum ozone greater than 60 ppb over the period May-September 2018 at AQS and CASTNet monitoring sites in the continental U.S. modeling domain.
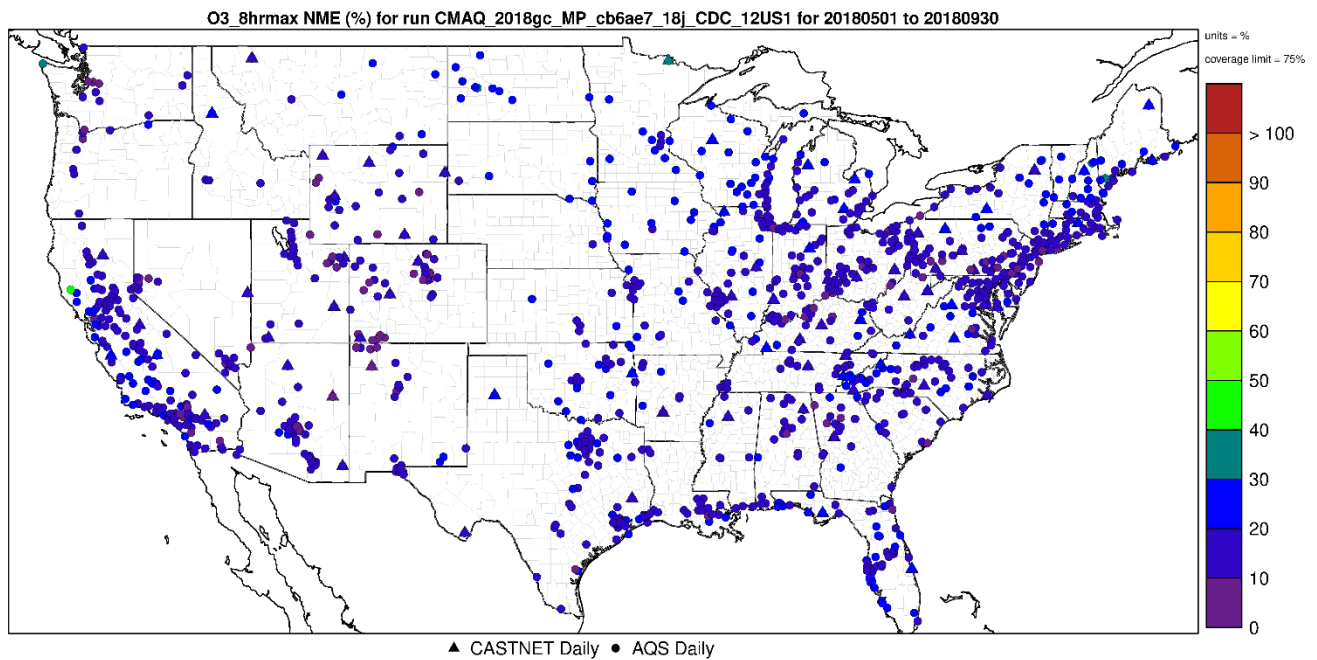
Figure 4-6. Normalized Mean Error (%) of 8-hour daily maximum ozone greater than 60 ppb over the period May-September 2018 at AQS and CASTNet monitoring sites in the continental U.S. modeling domain.

Evaluation for Annual PM₂.₅ 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 2018 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 over predicted at CASTNet, IMPROVE, and CSN monitoring sites across the 12-km modeling domain (with MB values ranging from 0.0 to -0.4 μgm^{-3}) except at CSN sites in the Upper Midwest, Northern Rockies and Northwest and at IMPROVE sites in the Upper Midwest and Northwest, as well as at CASTNet sites in the Northwest. Sulfate performance shows moderate error in the eastern subregions (average of approximately 30 percent) while Western subregions show slightly larger error (ranging from 32 to 60 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 and in the Upper Midwest with over predictions up to approximately 60 percent at individual monitors. Model error also shows a spatial trend by region, where much of the Eastern states are 10 to 40 percent, the Western and Central U.S. states are 20 to 100 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 -6 to -67 percent), except in the Northeast, Southeast, and Northwest where nitrate is over predicted (NMB in the range of approximately 5 to 23 percent). At IMPROVE rural sites, annual average nitrate is under predicted at all subregions, except in the Northeast (48.5 percent) and Southeast (8.2 percent) where nitrate is over predicted. Likewise, model performance of total nitrate at sub-urban CASTNet monitoring sites shows an under prediction at all subregions (NMB in the range of -0.5 to -47.4 percent) except in the Northeast (NMB 10.9 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 over prediction of greater than 20 percent at most monitoring sites along the Northeast and Northwest coastline as well as in the Southeast as indicated in Figure 4-13. The exception to this is in the Ohio Valley, South, Southwest, Northern Rockies 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.

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 -13.8 to -74.8 percent). Ammonium performance across the urban CSN sites shows an under prediction in three of the climate subregions (South, Southwest and West ranging from -13.6 to -69.5 percent), except in the Northeast, Ohio Valley, Upper Midwest, Southeast, Northwest, and Northern Rockies (over prediction of NMB). 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 Northeast and in the Northern

Rockies, (over prediction bias on average 80 to 100 percent). The urban monitoring sites exhibit larger errors than at rural sites for ammonium.

Annual average elemental carbon is under predicted in all of the nine climate regions at urban and rural sites (biases between -15.4 to 52.9 percent). 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 1.3 to 69.3 percent), except in the Northern Rockies and West where the NMB ranges from -5.9 to -16.6 percent. The model over predicted annual average organic carbon in all subregions at urban CSN sites except in the Northern Rockies (NMB approximately -21 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 2018 Annual PM Species Model Performance Statistics by NOAA Climate region, by Monitoring Network.

Pollutant	Monitor Network	Subregion	No. of Obs	MB (µgm⁻³)	ME (µgm⁻³)	NMB (%)	NME (%)
	CSN	Northeast	2,797	0.0	0.3	-4.1	34.6
		Ohio Valley	2,035	-0.1	0.4	-7.9	33.1
		Upper Midwest	1,108	0.1	0.3	11.8	38.5
		Southeast	1,555	-0.1	0.3	-12.9	30.5
		South	1,253	-0.2	0.5	-13.3	36.1
		Southwest	902	-0.1	0.2	-26.9	45.3
		Northern Rockies	589	0.1	0.3	15.8	45.9
		Northwest	604	0.1	0.1	28.9	56.4
		West	1,152	-0.4	0.5	-38.1	51.2
	IMPROVE	Northeast	1,783	-0.1	0.2	-10.6	32.2
		Ohio Valley	871	-0.2	0.4	-20.0	33.2
		Upper Midwest	944	0.0	0.2	5.3	35.9
		Southeast	1,480	-0.2	0.3	-24.8	34.3
Sulfate		South	1,012	-0.2	0.4	-20.3	36.9
		Southwest	3,749	-0.1	0.2	-33.2	47.4
		Northern Rockies	2,275	0.0	0.2	-7.1	39.0
		Northwest	1,934	0.1	0.2	31.3	60.8
		West	2,463	-0.2	0.3	-30.8	50.9
	CASTNet	Northeast	898	-0.2	0.2	-21.5	26.9
		Ohio Valley	872	-0.3	0.3	-25.2	26.7
		Upper Midwest	241	-0.1	0.2	-10.5	21.6
		Southeast	558	-0.4	0.4	-34.2	36.1
		South	388	-0.4	0.4	-30.1	32.0
		Southwest	445	-0.1	0.2	-33.8	41.0
		Northern Rockies	529	-0.1	0.1	-22.8	32.0
		Northwest	51	0.1	0.1	18.4	32.2
		West	294	-0.3	0.3	-48.5	53.7
	CSN	Northeast	2,797	0.0	0.5	4.8	54.6
		Ohio Valley	2,035	-0.2	0.6	-12.9	45.5
		Upper Midwest	1,245	-0.1	0.5	-6.2	43.9
		Southeast	1,909	0.1	0.3	22.7	80.0
		South	1,252	-0.1	0.4	-14.6	71.6
Nitrate		Southwest	902	-0.4	0.6	-53.9	75.8
		Northern Rockies	587	-0.3	0.5	-31.2	57.8
		Northwest	604	0.1	0.6	9.8	89.4
		West	1,152	-1.6	1.7	-67.0	71.8
	IMPROVE	Northeast	1,782	0.2	0.3	48.5	88.4

Pollutant	Monitor Network	Subregion	No. of Obs	MB (µgm^{-3})	ME (µgm^{-3})	NMB (%)	NME (%)
		Ohio Valley	956	-0.3	0.3	-47.3	57.2
		Upper Midwest	870	-0.1	0.4	-16.5	55.4
		Southeast	1,477	0.0	0.3	8.2	77.9
		South	1,012	-0.1	0.4	-23.3	63.7
		Southwest	3,749	-0.2	0.2	-73.8	86.0
		Northern Rockies	2,273	-0.1	0.2	-40.8	79.7
		Northwest	1,921	-0.1	0.2	-26.6	96.0
		West	2,463	-0.3	0.3	-53.5	70.4
Total Nitrate (NO$_3$+HNO$_3$)	CASTNet	Northeast	898	0.1	0.3	10.9	31.3
		Ohio Valley	872	0.0	0.5	-0.5	26.6
		Upper Midwest	241	-0.2	0.4	-10.2	25.0
		Southeast	558	-0.1	0.5	-6.3	45.7
		South	388	-0.2	0.5	-17.8	35.6
		Southwest	445	-0.2	0.2	-25.8	37.3
		Northern Rockies	529	-0.2	0.2	-25.5	37.4
		Northwest	--	--	--	--	--
		West	294	-0.6	0.7	-47.4	50.5
Ammonium	CSN	Northeast	2,797	0.1	0.3	31.3	70.7
		Ohio Valley	2,036	0.0	0.3	1.0	51.3
		Upper Midwest	1,107	0.1	0.2	23.8	56.6
		Southeast	1,556	0.0	0.2	4.2	70.0
		South	1,253	-0.1	0.2	-13.6	63.2
		Southwest	902	-0.1	0.2	-59.2	78.0
		Northern Rockies	589	0.0	0.2	16.8	66.6
		Northwest	605	0.0	0.2	18.2	>100
		West	1,152	-0.5	0.6	-69.5	79.2
	CASTNet	Northeast	898	-0.1	0.1	-13.8	33.4
		Ohio Valley	872	-0.1	0.2	-23.1	30.1
		Upper Midwest	241	-0.1	0.2	-19.4	30.5
		Southeast	558	-0.1	0.1	-23.6	41.3
		South	388	-0.1	0.2	-25.7	42.2
		Southwest	445	-0.1	0.1	-59.5	65.7
		Northern Rockies	529	-0.1	0.1	-53.8	58.2
		Northwest	51	-0.1	0.1	-60.3	64.9
		West	294	-0.2	0.2	-74.8	78.3
Elemental Carbon	CSN	Northeast	2,833	-0.1	0.3	-18.6	44.4
		Ohio Valley	2,016	-0.2	0.3	-31.3	41.6

| Pollutant	Monitor Network	Subregion	No. of Obs	MB (μgm^{-3})	ME (μgm^{-3})	NMB (%)	NME (%)
		Upper Midwest	1,187	-0.1	0.2	-19.6	48.2
		Southeast	1,584	-0.2	0.2	-30.1	42.6
		South	1,148	-0.1	0.2	-18.1	39.1
		Southwest	850	-0.1	0.2	-20.6	40.5
		Northern Rockies	520	-0.2	0.2	-52.9	65.5
		Northwest	607	-0.1	0.4	-15.4	51.2
		West	1,124	-0.2	0.3	-22.7	38.1
	IMPROVE	Northeast	1,834	0.0	0.1	-16.2	41.9
		Ohio Valley	939	-0.1	0.1	-36.2	45.4
		Upper Midwest	1,050	-0.1	0.1	-25.2	51.9
		Southeast	1,612	-0.1	0.1	-37.6	46.0
		South	1,009	-0.1	0.1	-37.6	47.6
		Southwest	3,680	-0.1	0.1	-46.9	57.8
		Northern Rockies	2,317	-0.1	0.1	-40.0	61.4
		Northwest	1,860	-0.1	0.2	-30.6	72.1
		West	2,369	-0.1	0.2	-32.4	64.9
	CSN	Northeast	2,833	1.1	1.3	61.9	74.2
		Ohio Valley	2,017	0.6	1.1	32.7	55.4
		Upper Midwest	1,186	0.8	1.4	47.4	77.5
		Southeast	1,585	0.8	1.1	36.0	49.4
		South	1,150	0.8	1.3	45.6	68.5
		Southwest	850	0.3	1.0	17.2	56.4
		Northern Rockies	520	-0.3	1.1	-20.8	65.5
		Northwest	607	0.8	1.9	30.5	73.9
		West	1,124	0.2	1.3	5.9	41.7
Organic Carbon							
	IMPROVE	Northeast	1,843	0.7	0.9	69.3	87.1
		Ohio Valley	942	0.6	1.1	32.7	55.4
		Upper Midwest	1,050	0.7	1.1	68.5	>100
		Southeast	1,618	0.6	0.8	48.3	61.4
		South	1,011	0.6	0.8	46.1	71.2
		Southwest	3,720	0.0	0.5	2.5	63.4
		Northern Rockies	2,382	-0.2	0.8	-16.6	65.6
		Northwest	1,915	0.0	1.4	1.3	81.1
		West	2,428	0.2	1.3	-5.9	69.6

SO4 MB (ug/m3) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231
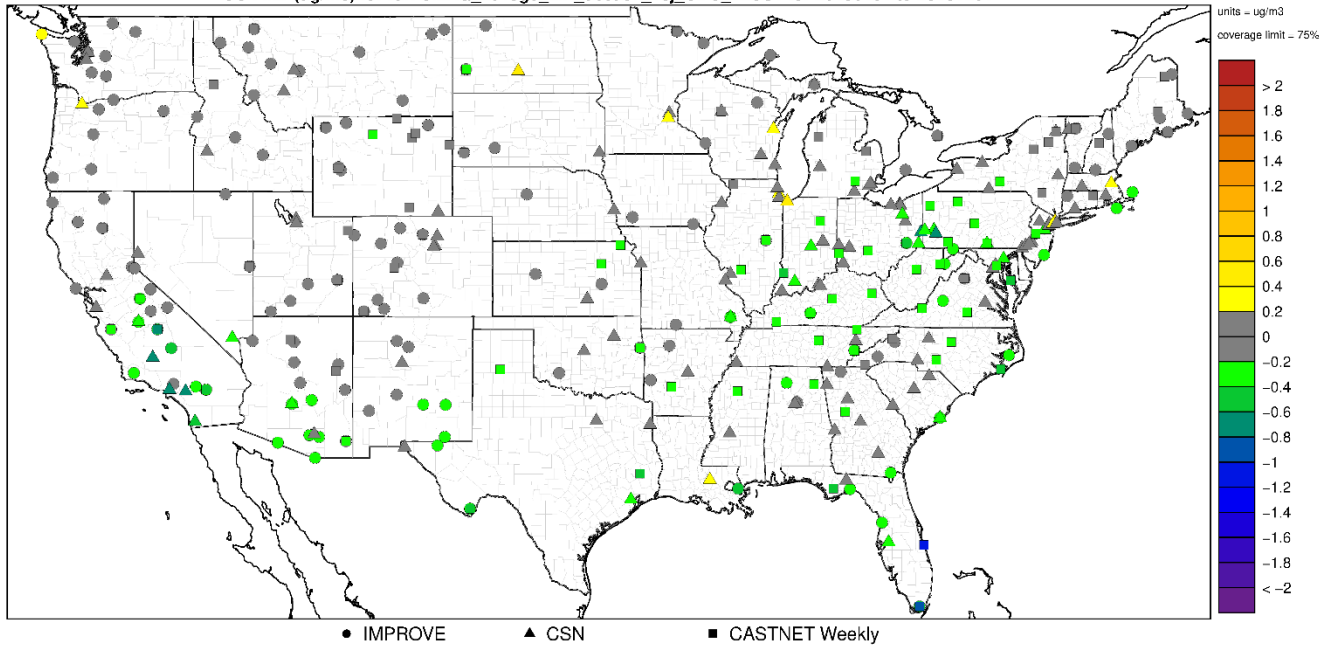
SO4 ME (ug/m3) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231

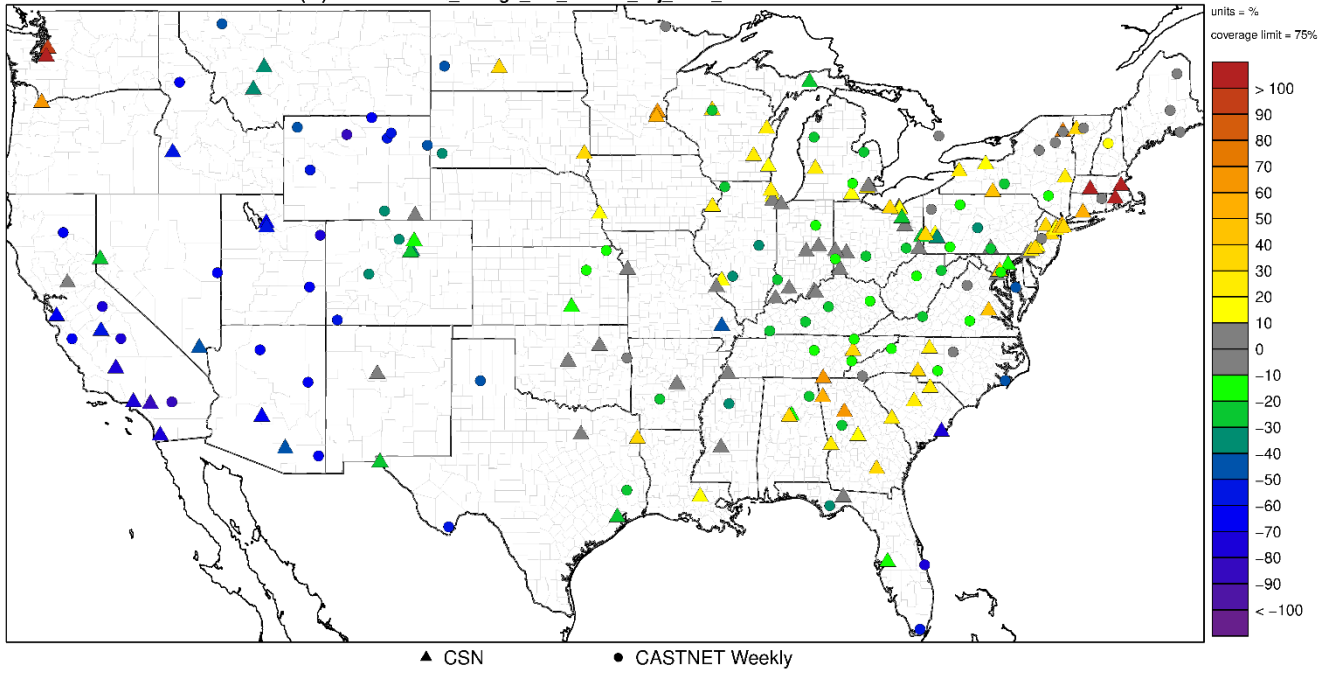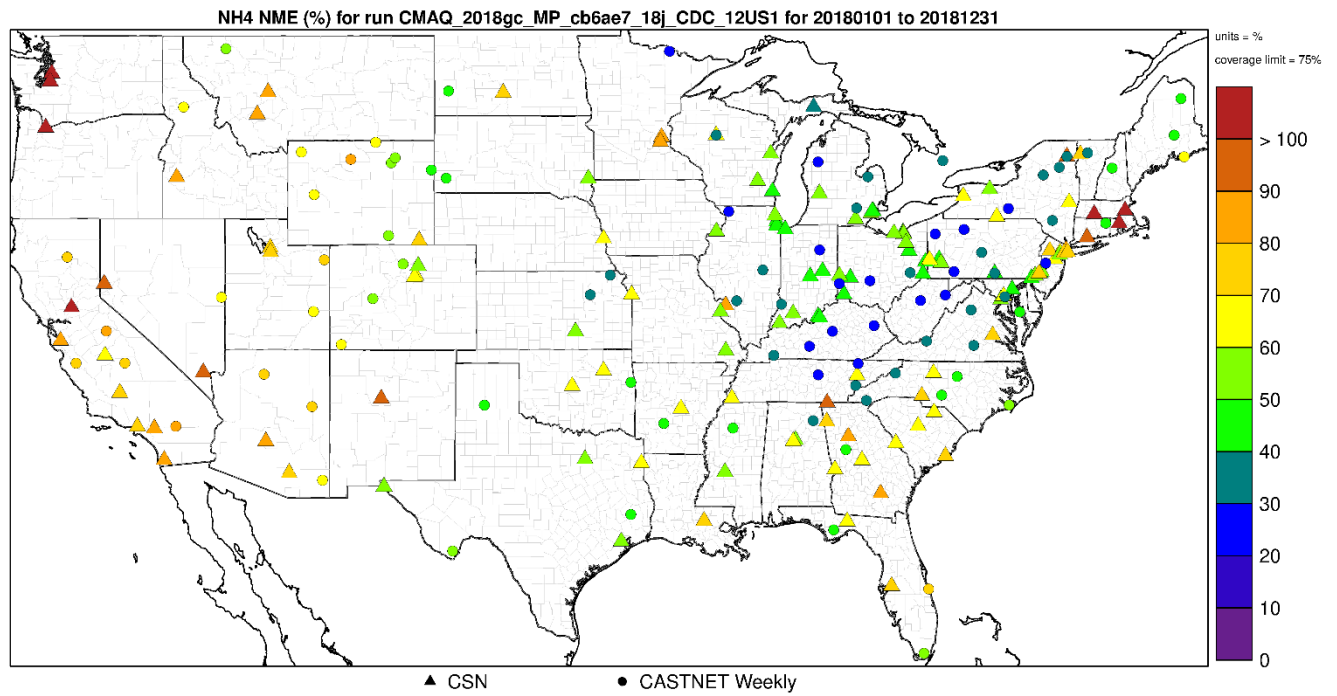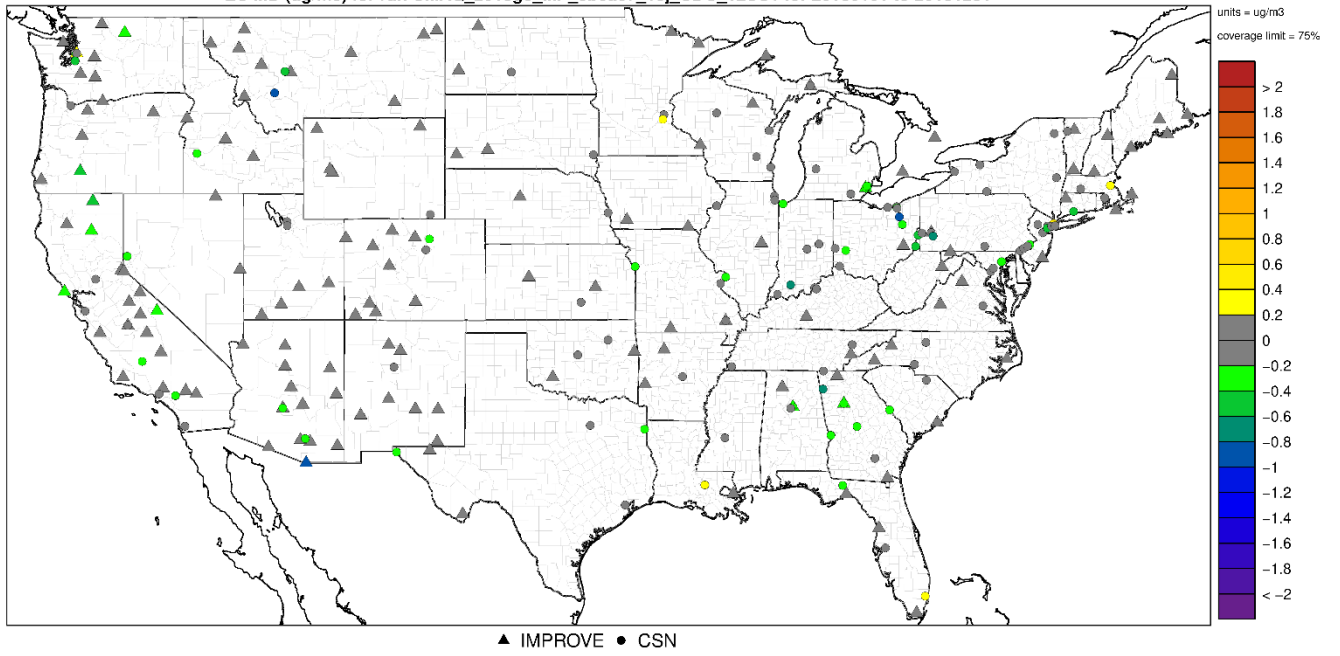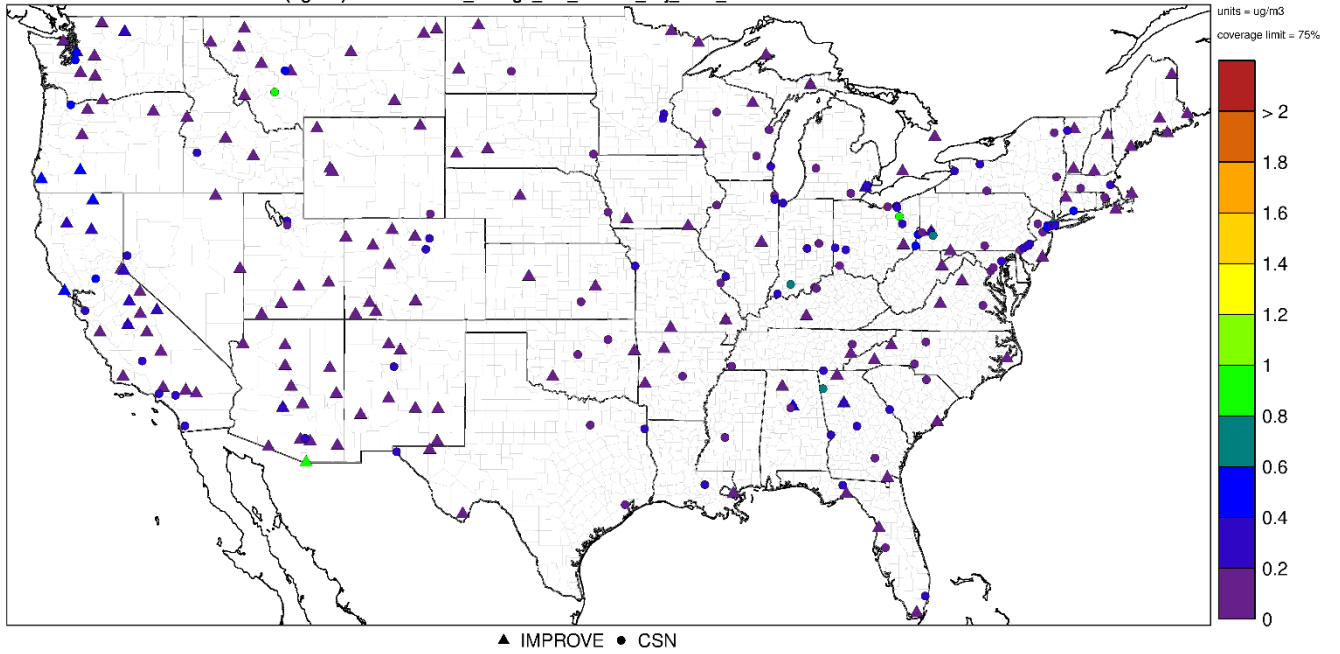SO4 NMB (%) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231

● IMPROVE   ▲ CSN   ■ CASTNET Weekly

SO4 NME (%) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231
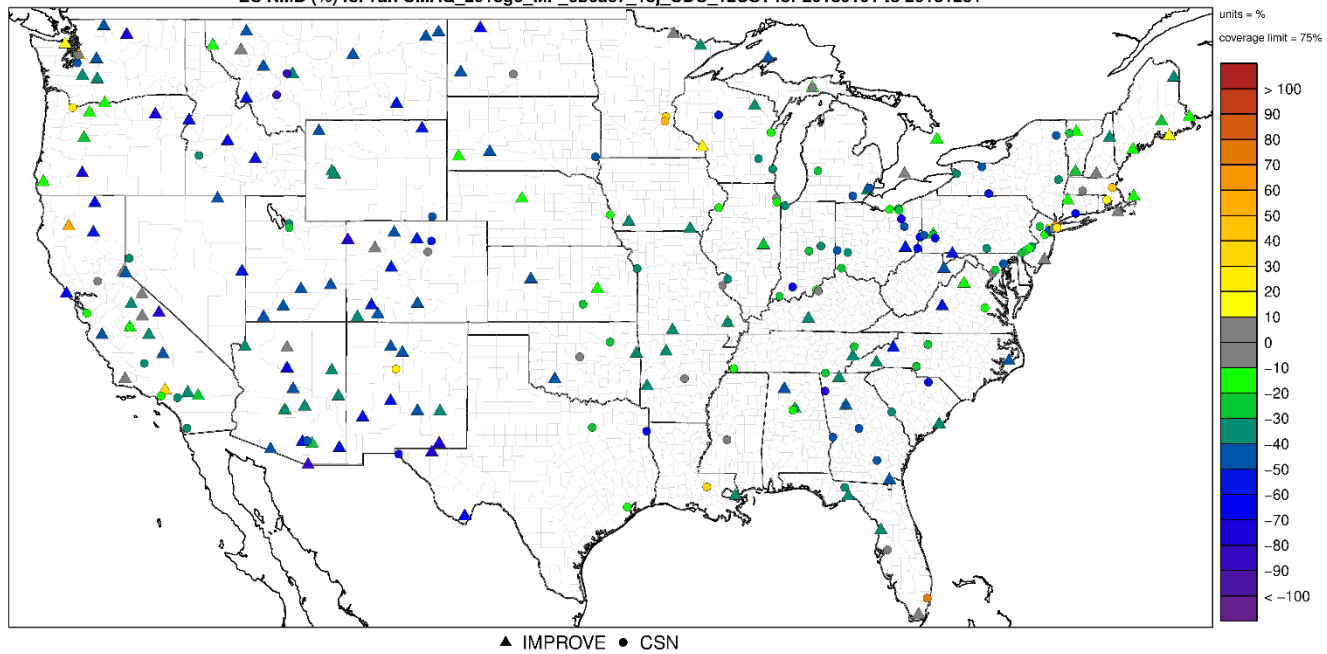
● IMPROVE   ▲ CSN   ■ CASTNET Weekly
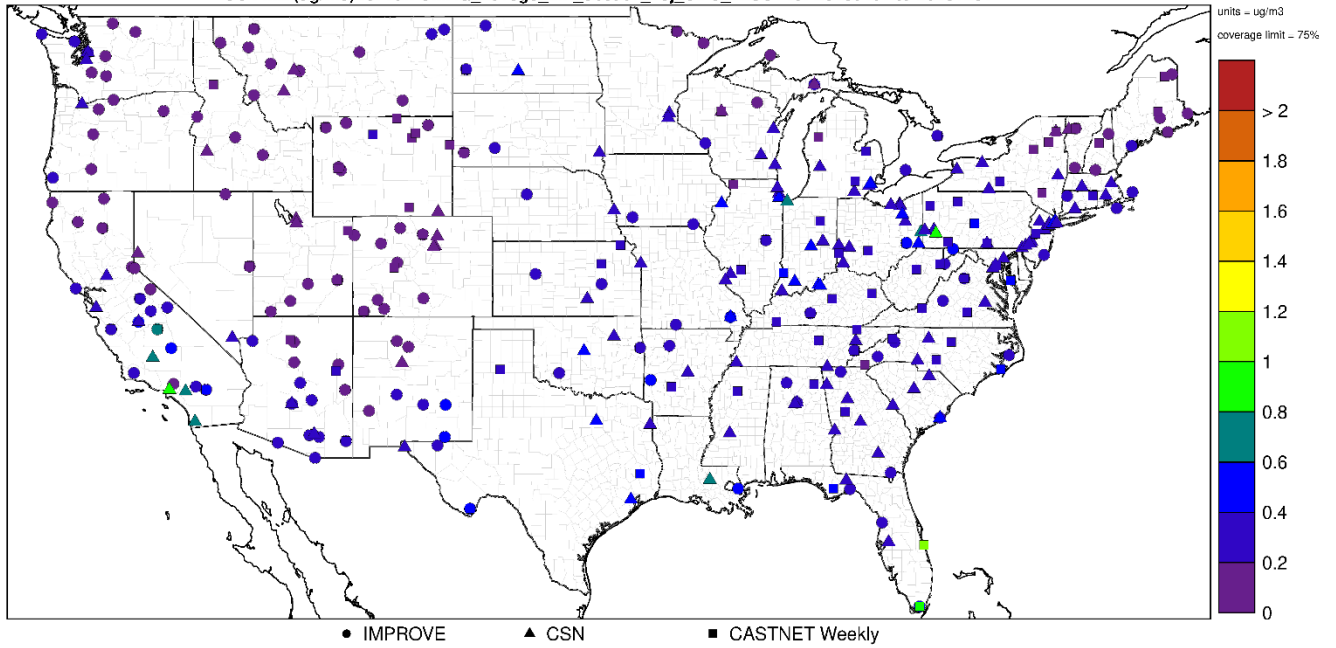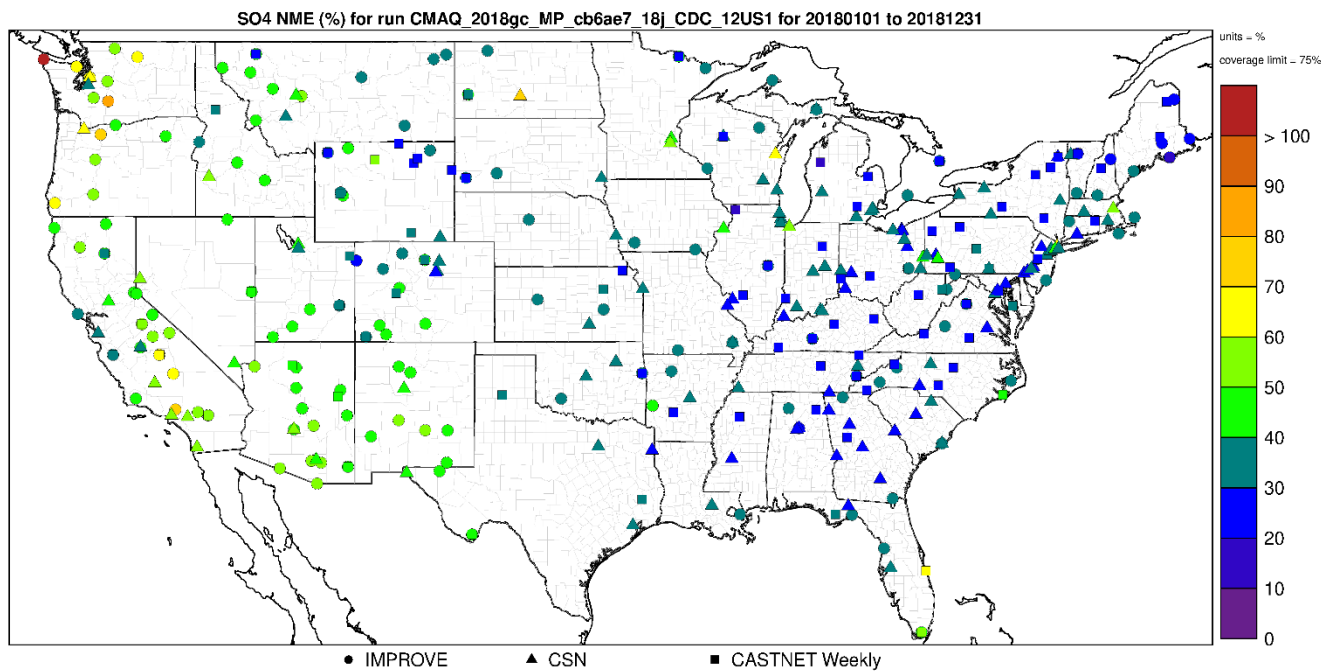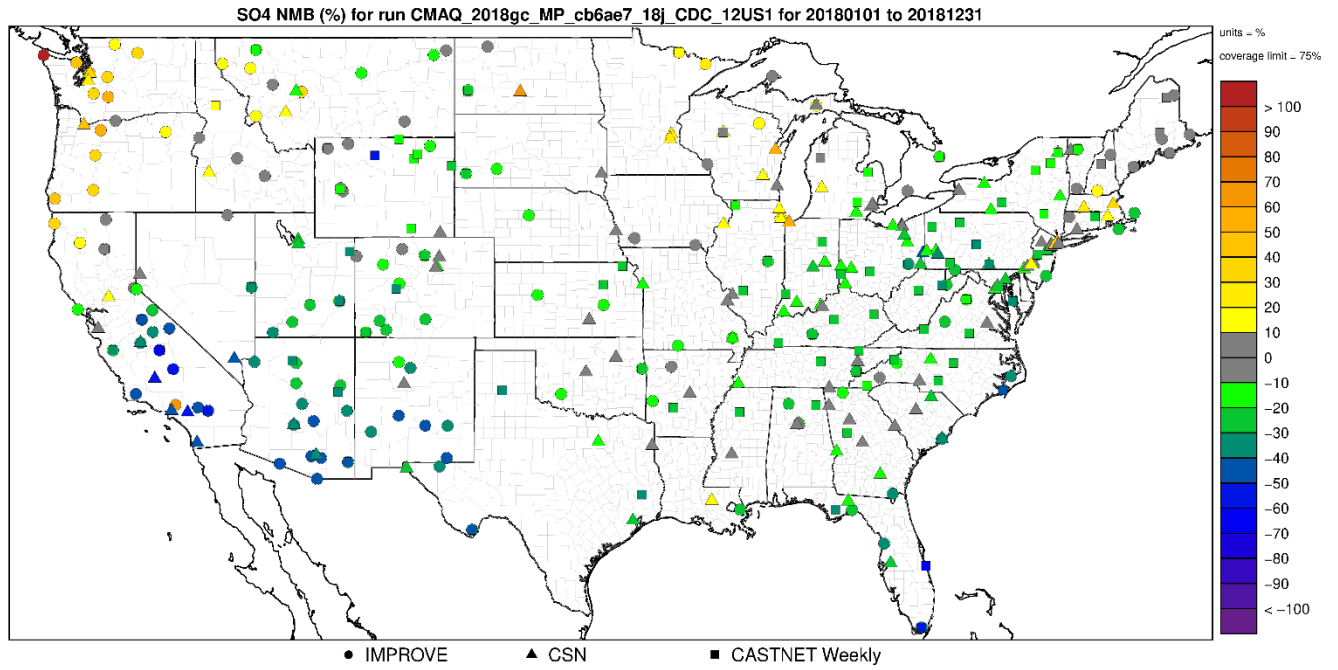
NO3 MB (ug/m3) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231

NO3 ME (ug/m3) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231

NO3 NMB (%) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231
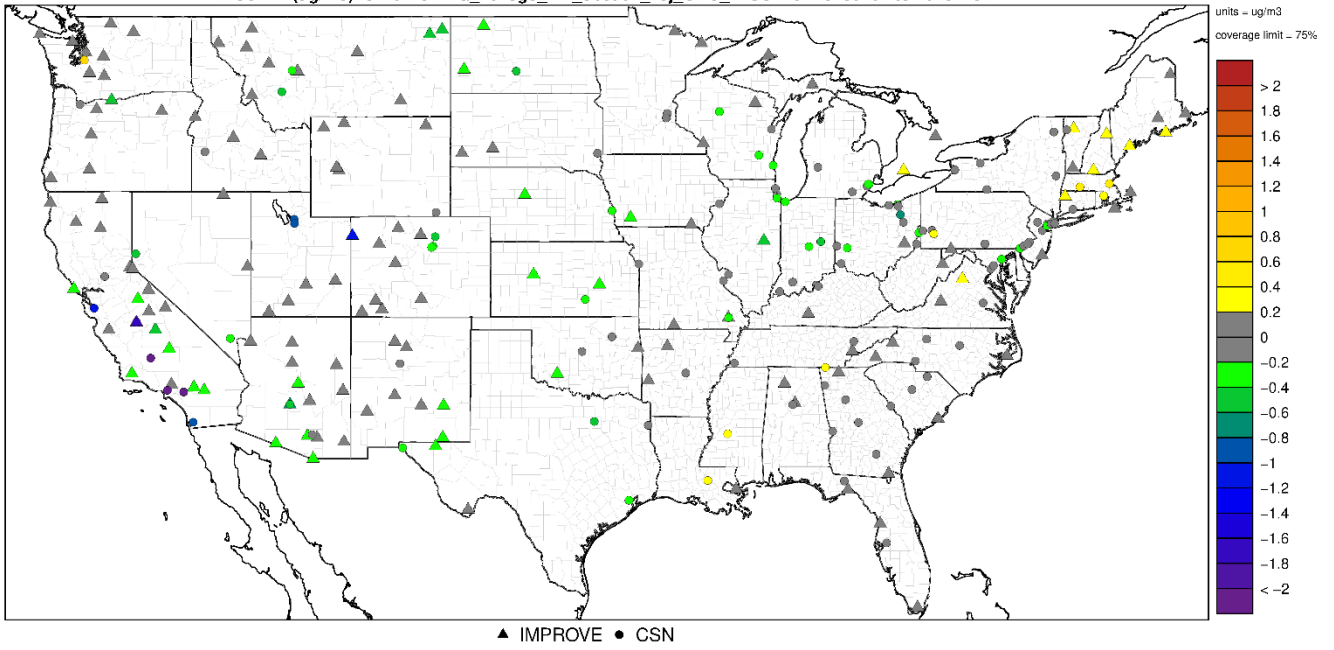
NO3 NME (%) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231
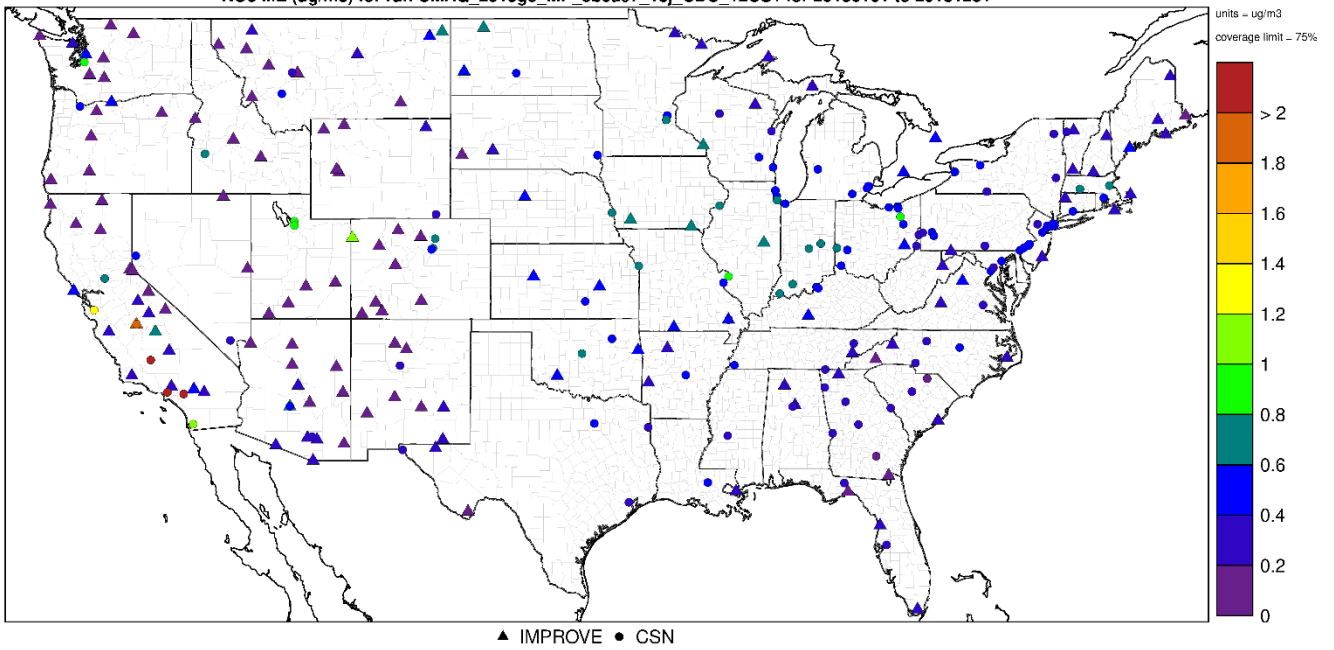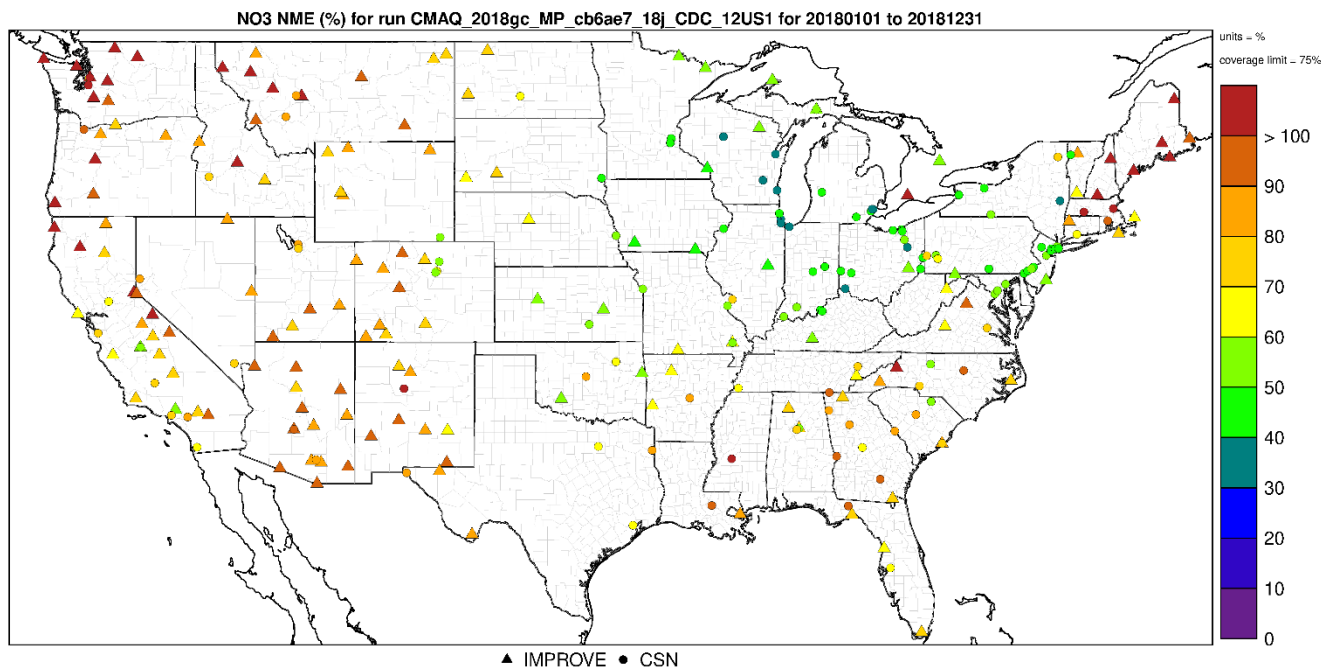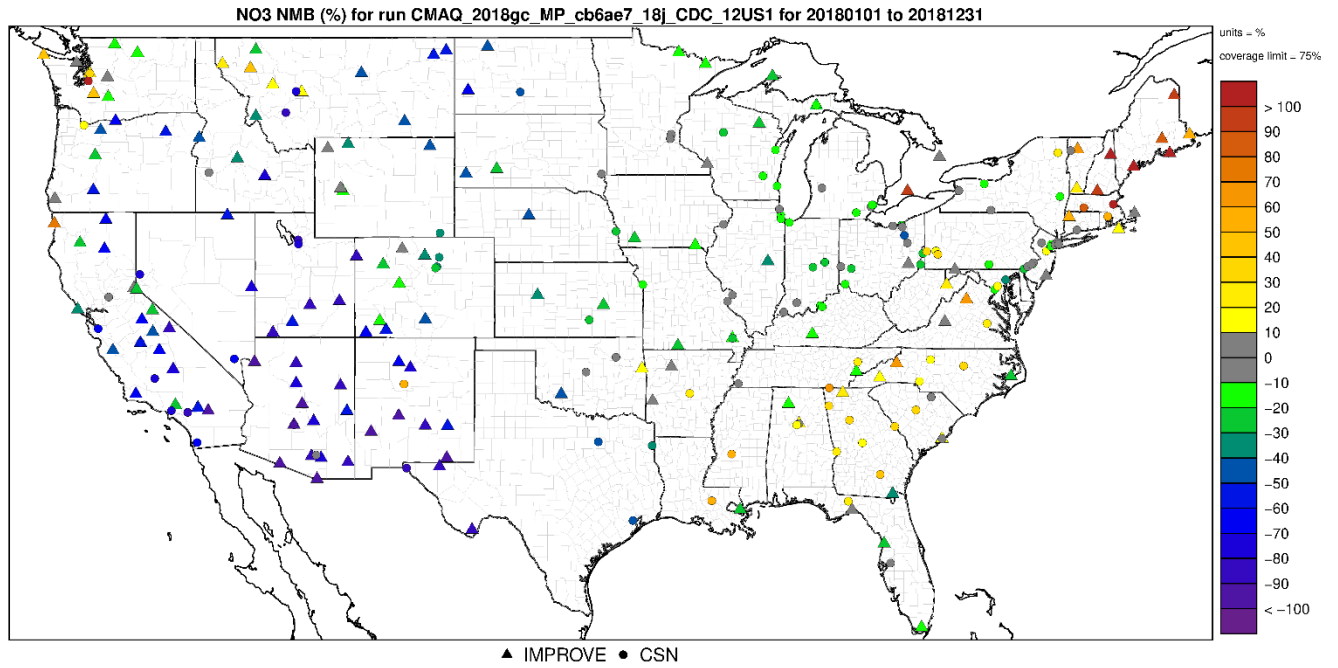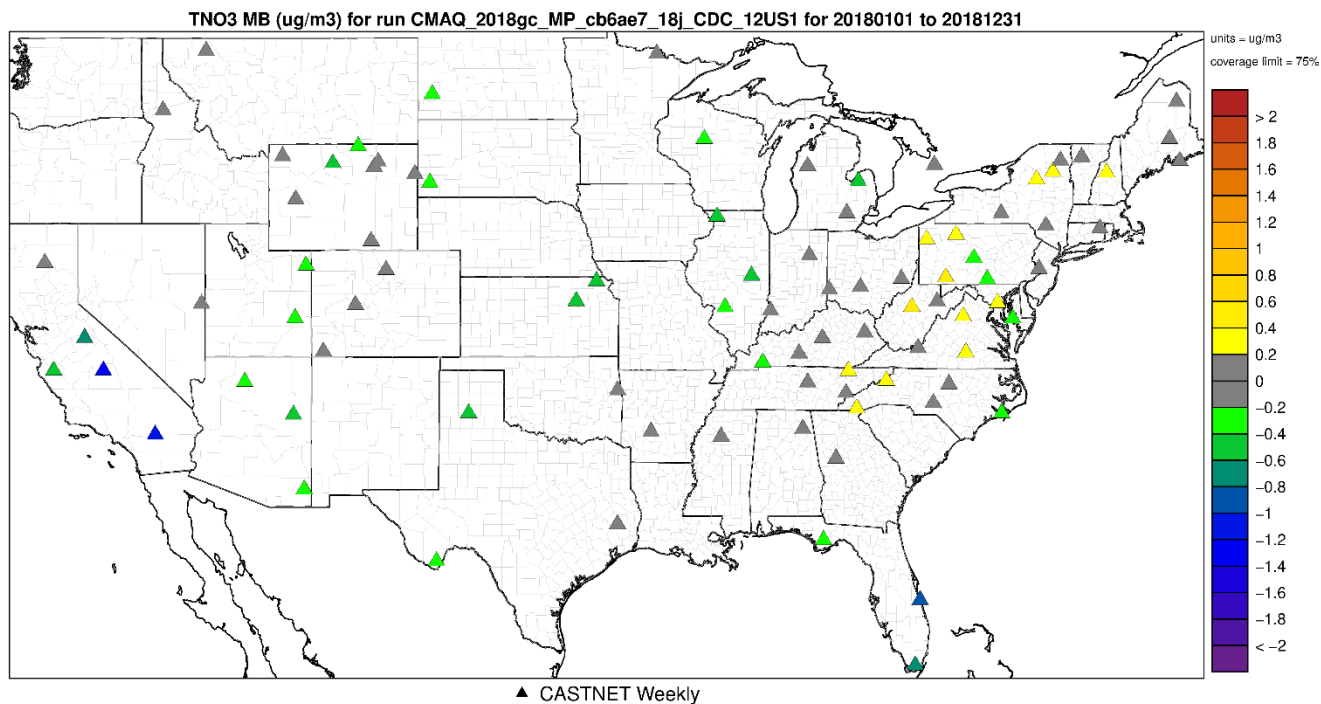
Figure 4-15. Mean Bias (μgm⁻³) of annual total nitrate at monitoring sites in the continental U.S. modeling domain.
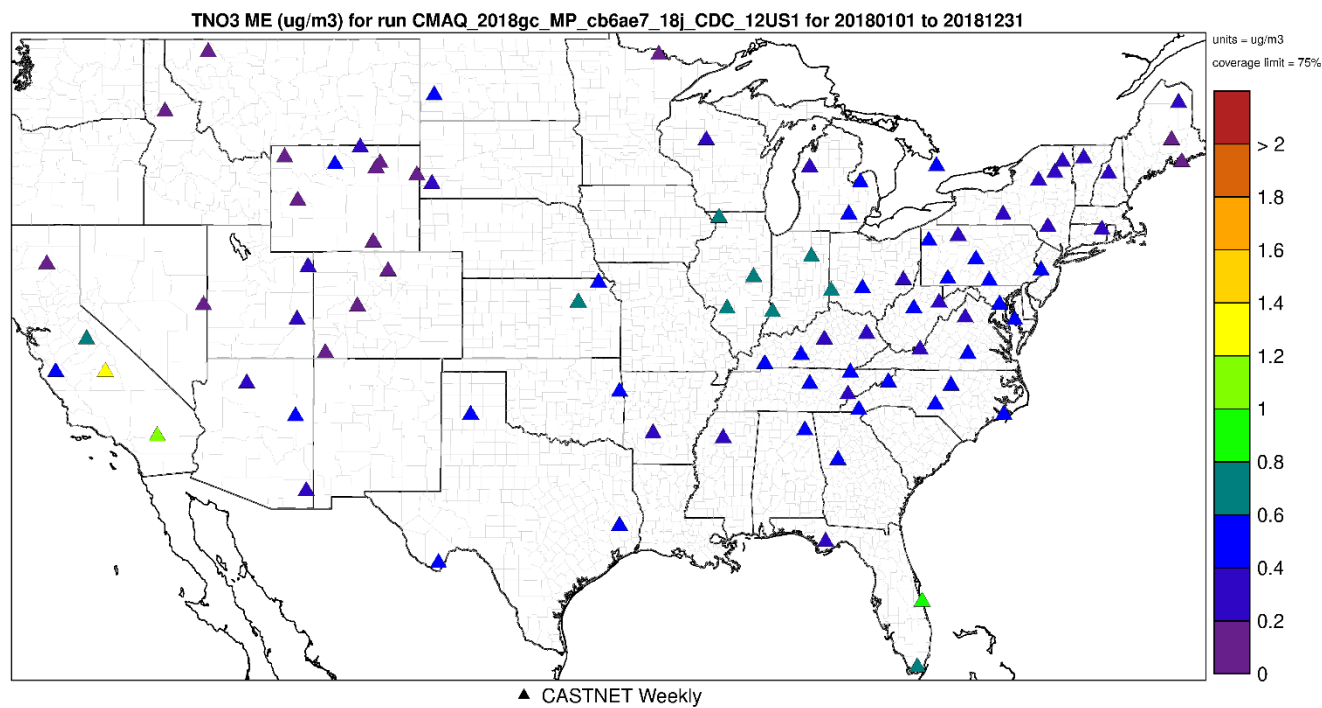
**Figure 4-16. Mean Error (µgm⁻³) of annual total nitrate at monitoring sites in the continental U.S. modeling domain.**

TNO3 NMB (%) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231
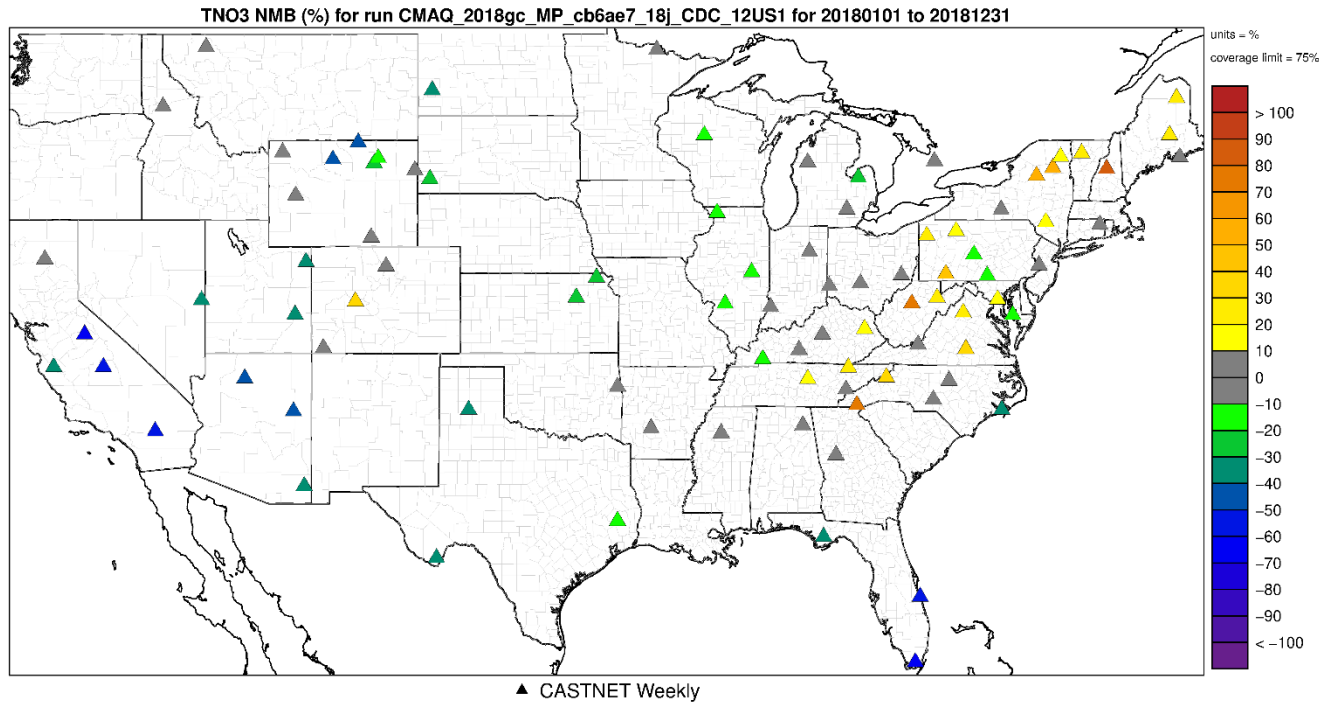
▲ CASTNET Weekly

TNO3 NME (%) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231

units = %
coverage limit = 75%
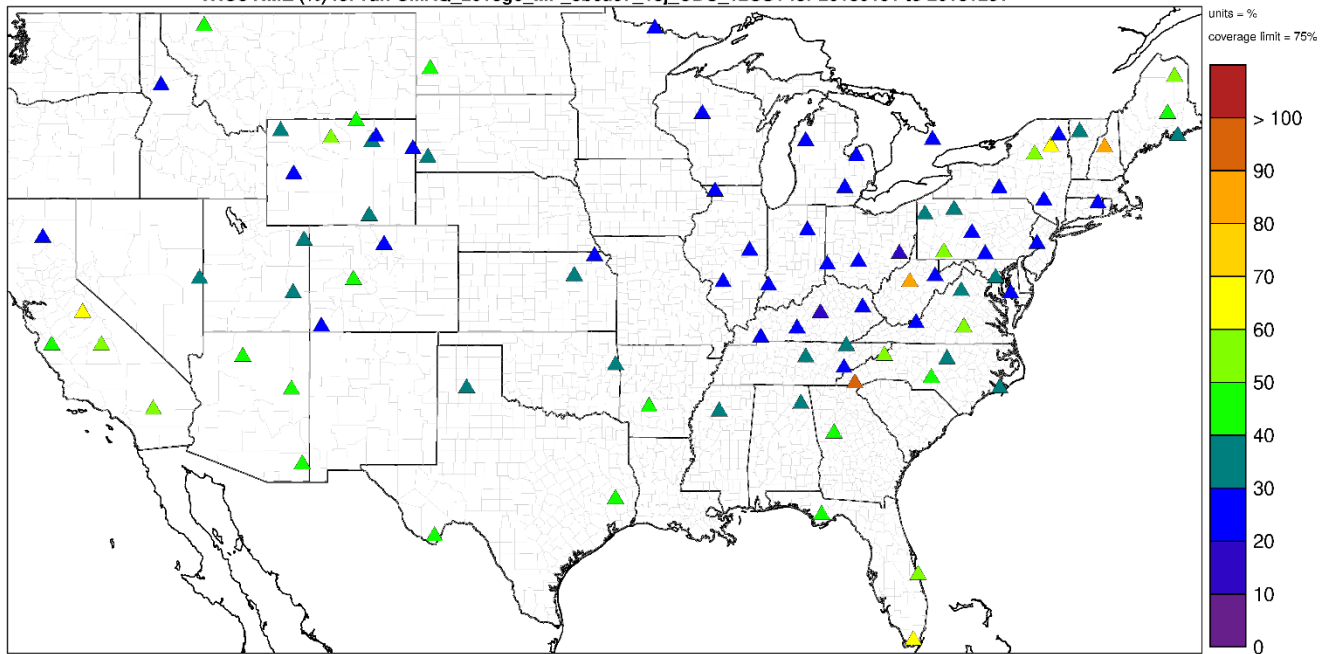
▲ CASTNET Weekly

NH4 MB (ug/m3) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231

units = ug/m3
coverage limit = 75%
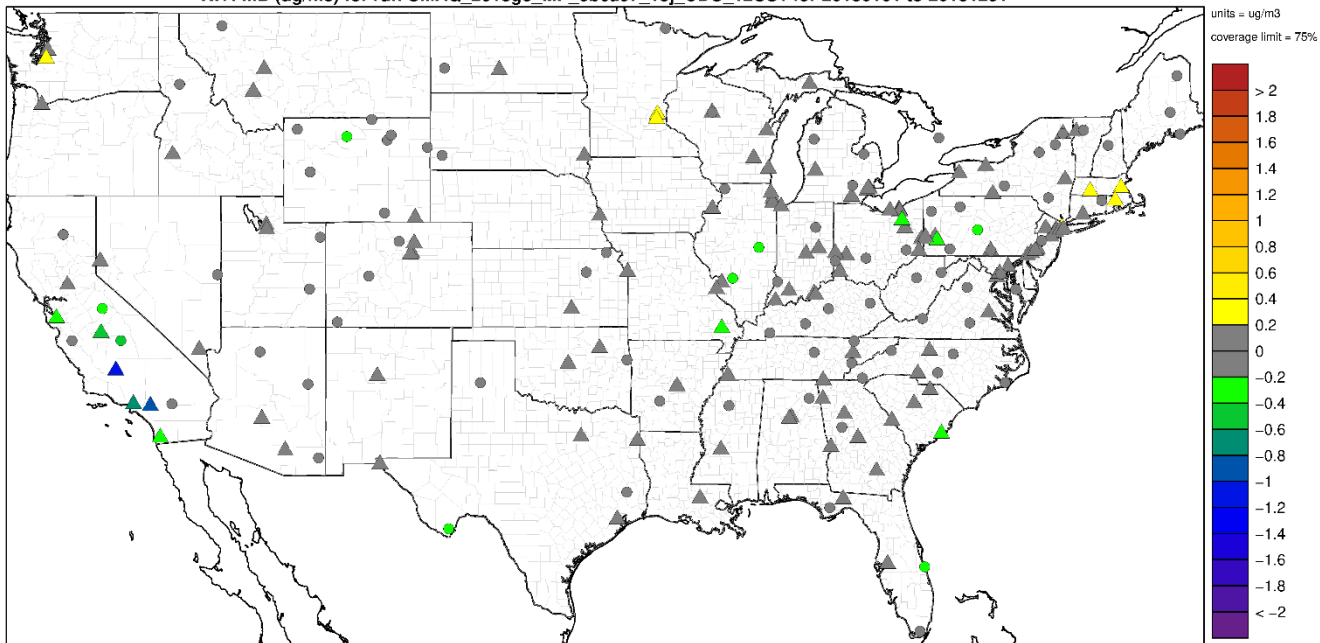
▲ CSN   ● CASTNET Weekly

NH4 ME (ug/m3) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231
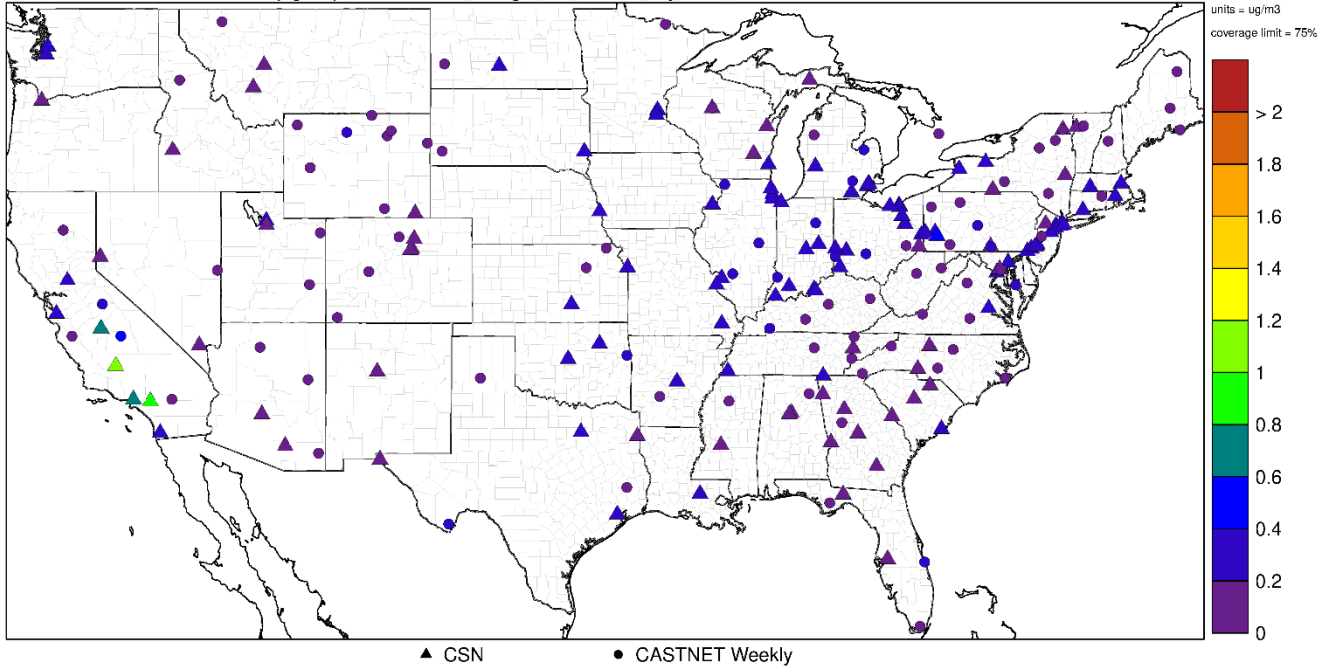
NH4 NMB (%) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231

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

NH4 NME (%) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231

EC MB (ug/m3) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231

▲ IMPROVE ● CSN

EC ME (ug/m3) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231

▲ IMPROVE ● CSN

EC NMB (%) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231

EC NME (%) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231

OC MB (ug/m3) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231

IMPROVE ● CSN

OC ME (ug/m3) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231

IMPROVE ● CSN

OC NMB (%) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231

▲ IMPROVE   ● CSN

OC NME (%) for run CMAQ_2018gc_MP_cb6ae7_18j_CDC_12US1 for 20180101 to 20181231

▲ IMPROVE   ● CSN
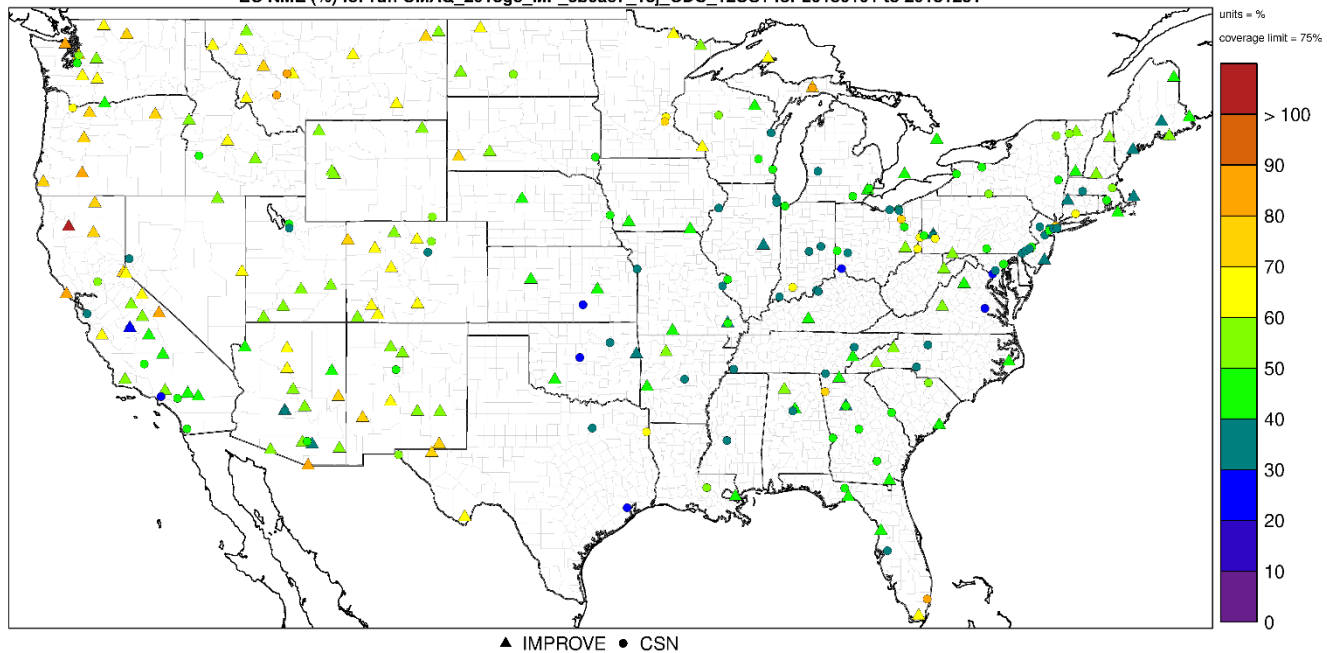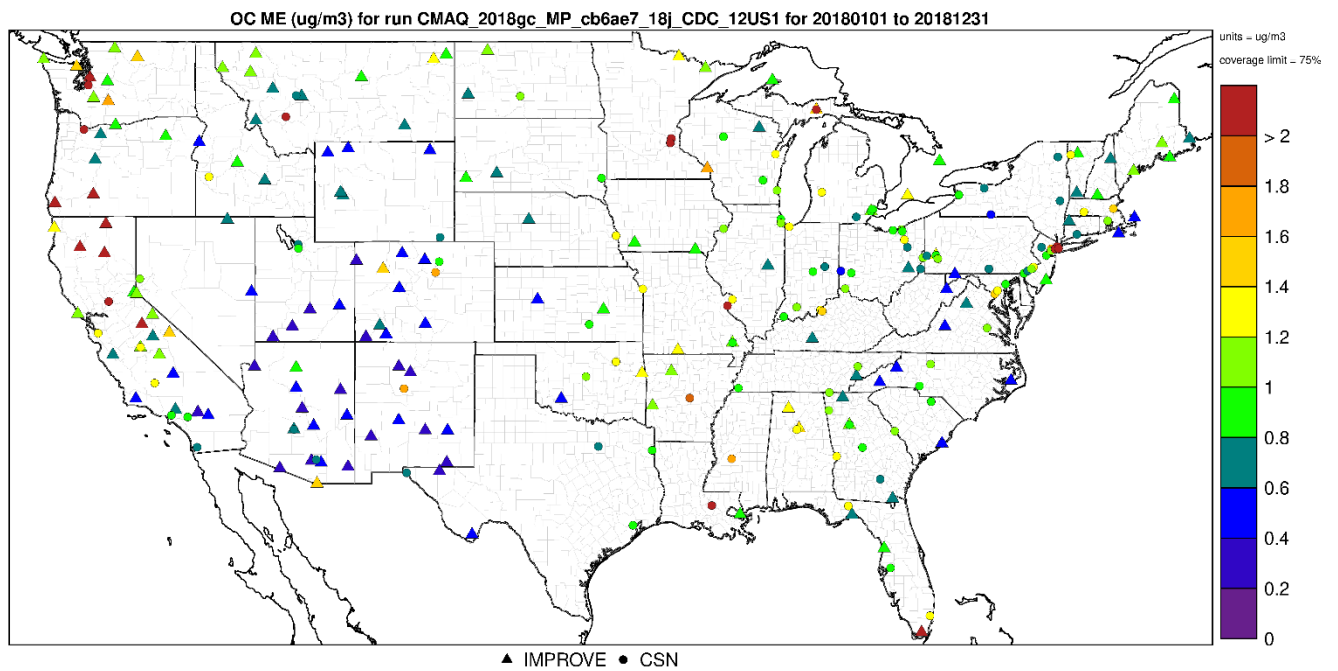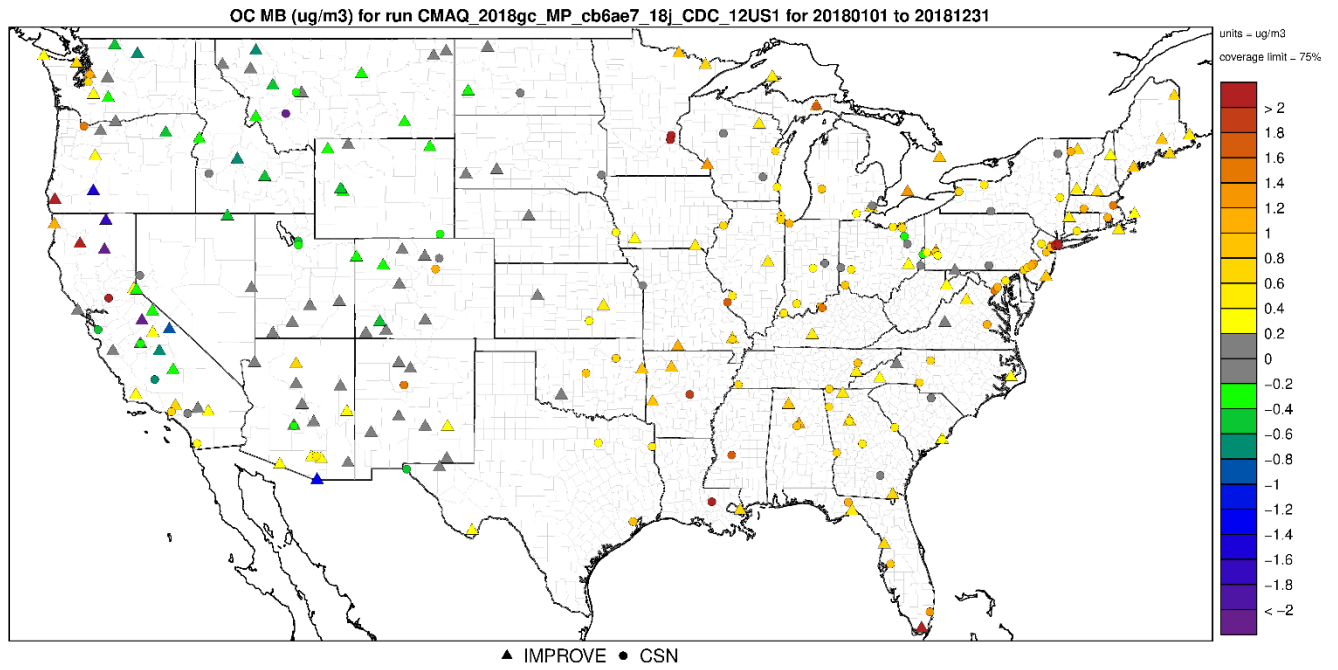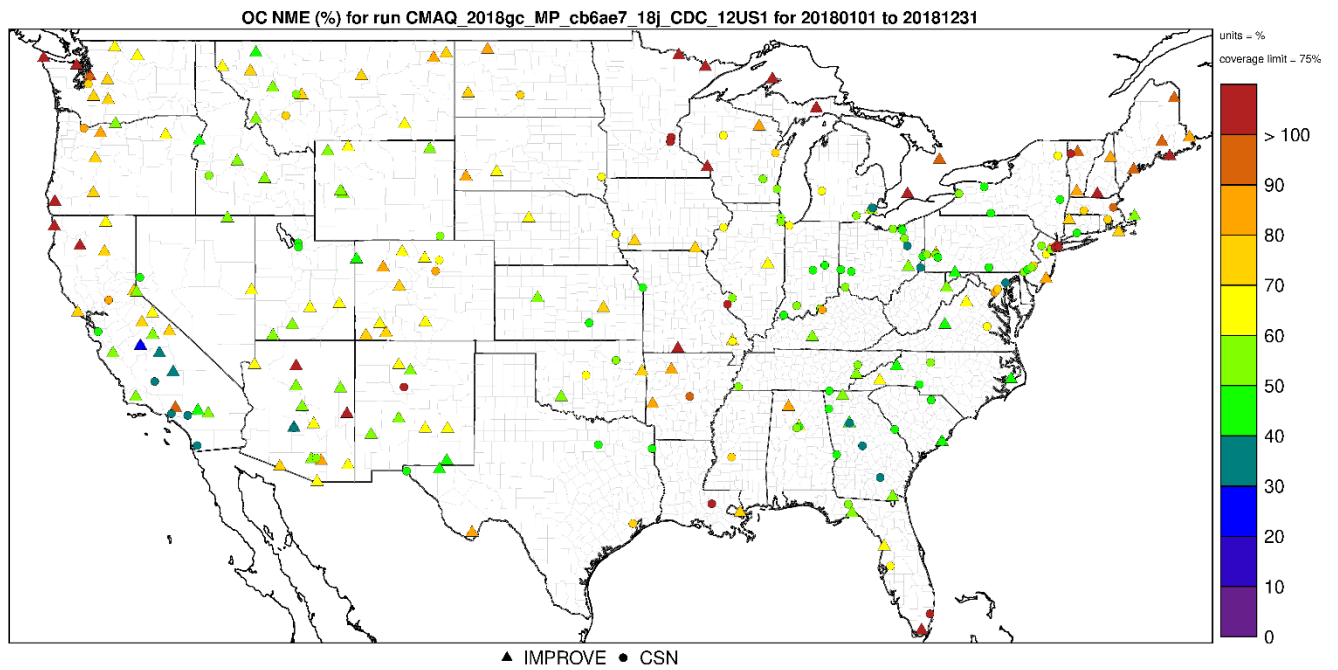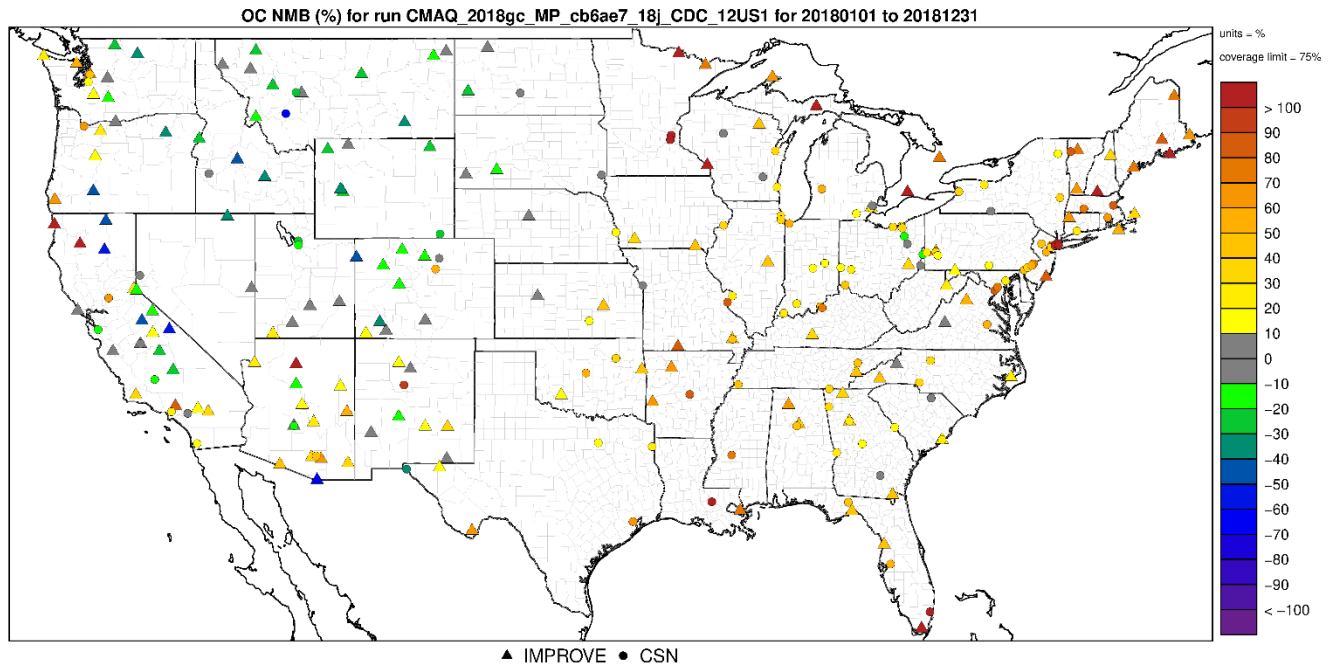
5.0 Bayesian space-time downscaling fusion model (downscaler) -Derived Air Quality Estimates

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 accuracy and CMAQs 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 PM2.5 data from AQS and CMAQ to produce predictions to continental U.S. 2010 census tract centroids for the year 2018.

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 PM2.5). 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 β_0 and a local component $\beta_0(s)$ that is modeled as a mean-zero Gaussian Process with exponential decay
β_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 $\widetilde{\beta}_0$ and β_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 (i.e., $\widetilde{\beta}_0(s)$, β_1, $\widetilde{x}(s)$) 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)[31] 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 2010 US census tract centroids across the continental U.S. using 2018 measurement and CMAQ data as inputs. For ozone, the concentration unit is the daily maximum 8-hour average in ppb and for PM2.5 the concentration unit is the 24-hour average in µg/m3.

5.3.1   Summary of 8-hour Ozone Results

Figure 5-1 summarizes the AQS, CMAQ and DS ozone data over the year 2018. It shows the 4th max daily maximum 8-hour average ozone for AQS observations, CMAQ model predictions and DS model results. The DS model estimated that for 2018, about 60% of the US Census tracts (43711 out of 72283) experienced at least one day with an ozone value above the NAAQS of 70 ppb.

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[31] 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.
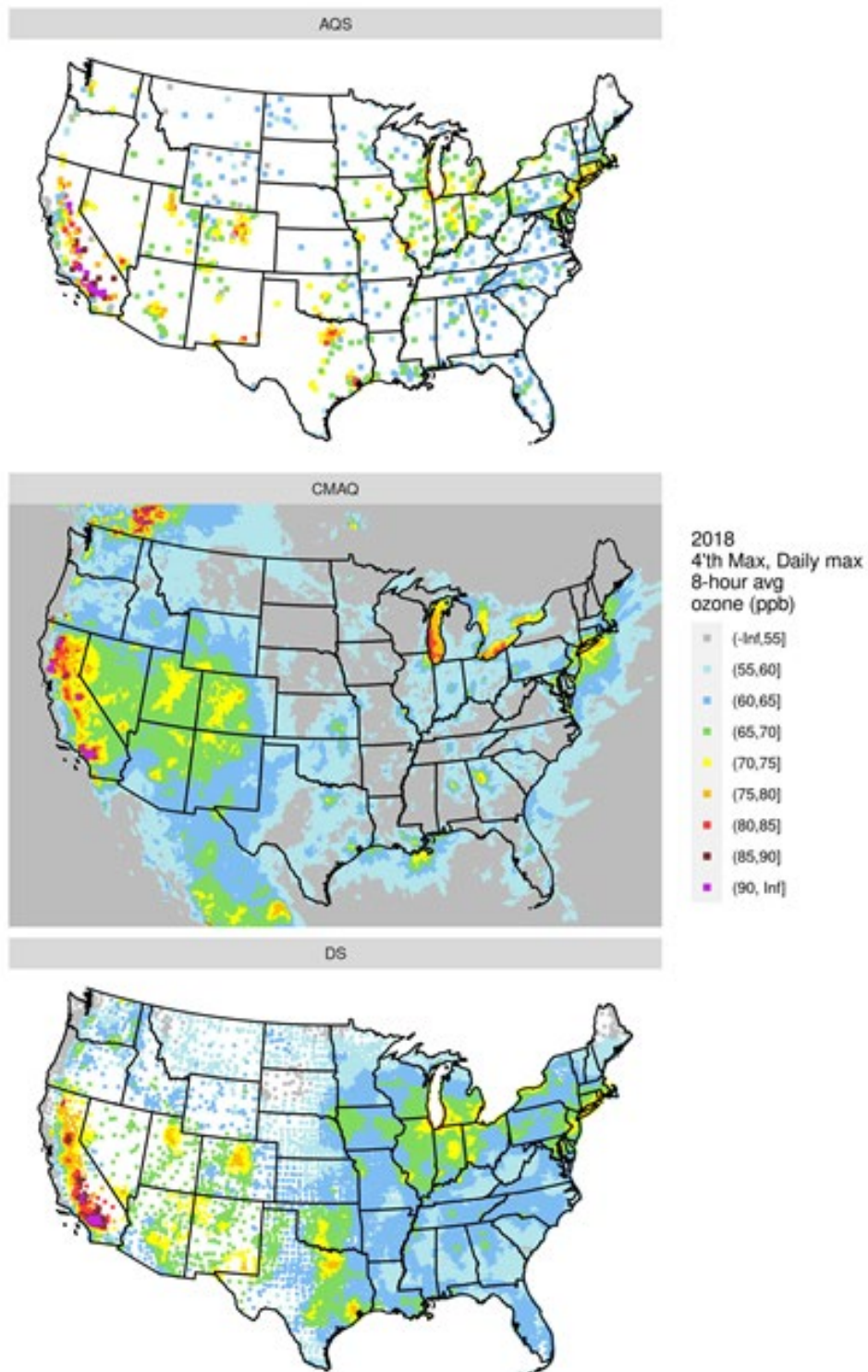
Figure 5-1. Annual 4th max (daily max 8-hour ozone concentrations) derived from AQS, CMAQ and DS data.

5.3.2 Summary of PM₂.₅ Results

Figures 5-2 and 5-3 summarize the AQS, CMAQ and DS PM2.5 data over the year 2018. Figure 5-2 shows annual means and Figure 5-3 shows 98th percentiles of 24-hour PM2.5 concentrations for AQS observations, CMAQ model predictions and DS model results. The DS model estimated that for 2018 about 23% of the US Census tracts (16372 out of 72283) experienced at least one day with a PM2.5 value above the 24-hour NAAQS of 35 μg/m3.
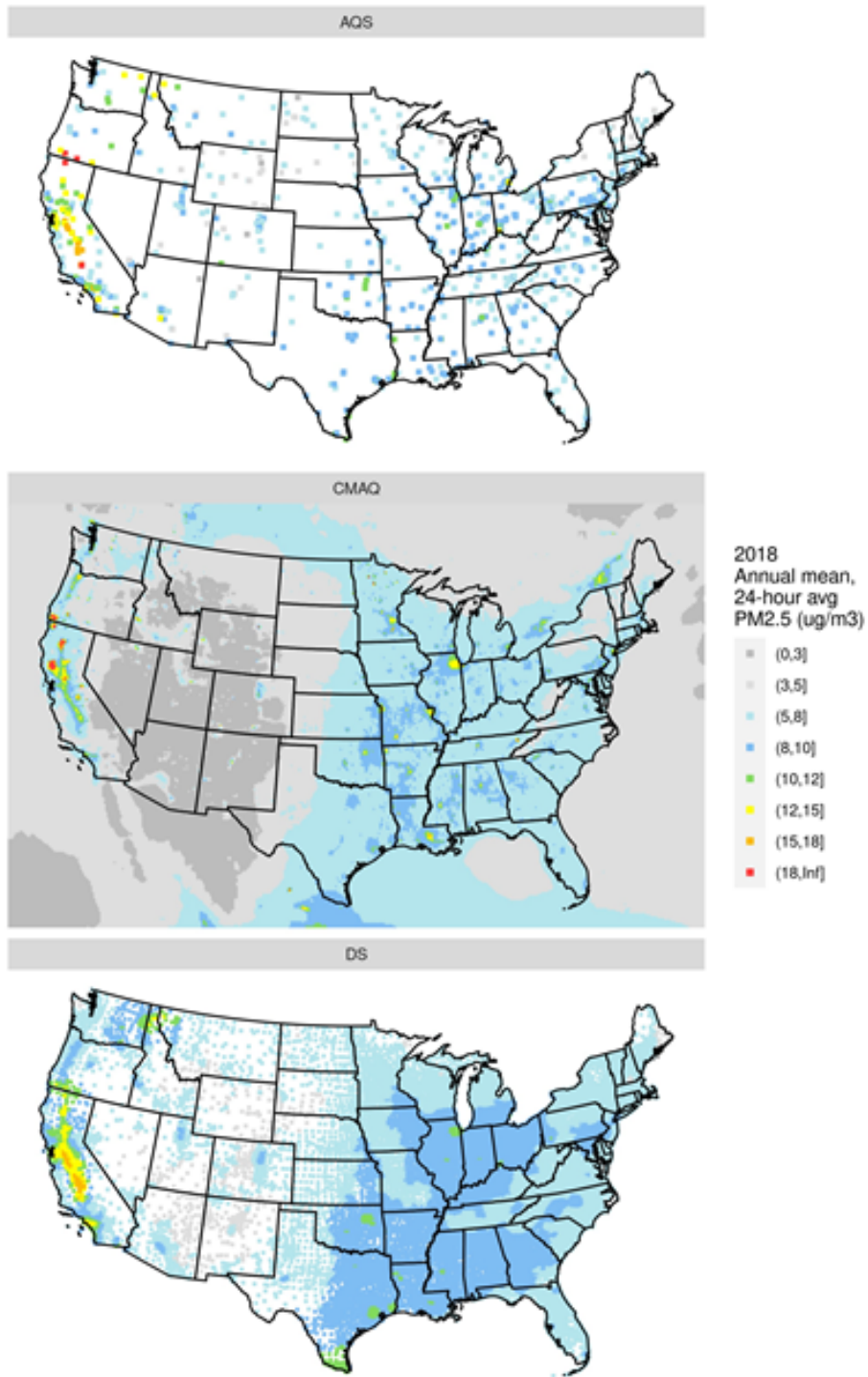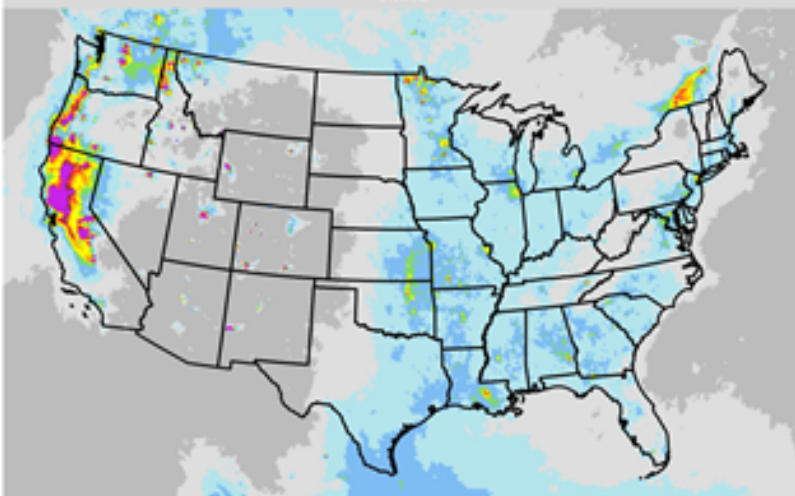
Figure 5-2. Annual mean PM$_{2.5}$ concentrations derived from AQS, CMAQ and DS data.

AQS

CMAQ

2018
98'th percentile,
24-hour avg
PM2.5 (ug/m3)

- (0,10]
- (10,15]
- (15,20]
- (20,25]
- (25,30]
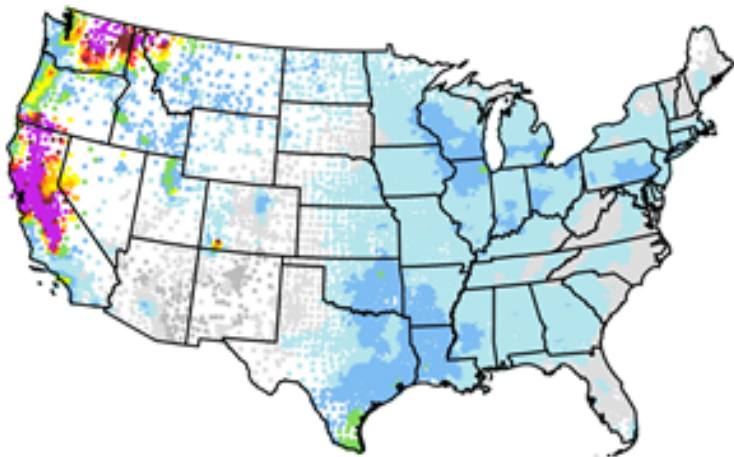- (30,35]
- (35,40]
- (40,45]
- (45,50]
- (50,Inf]

DS

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 (i.e., the eastern US), and larger in regions with more sparse monitoring networks (i.e., 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.
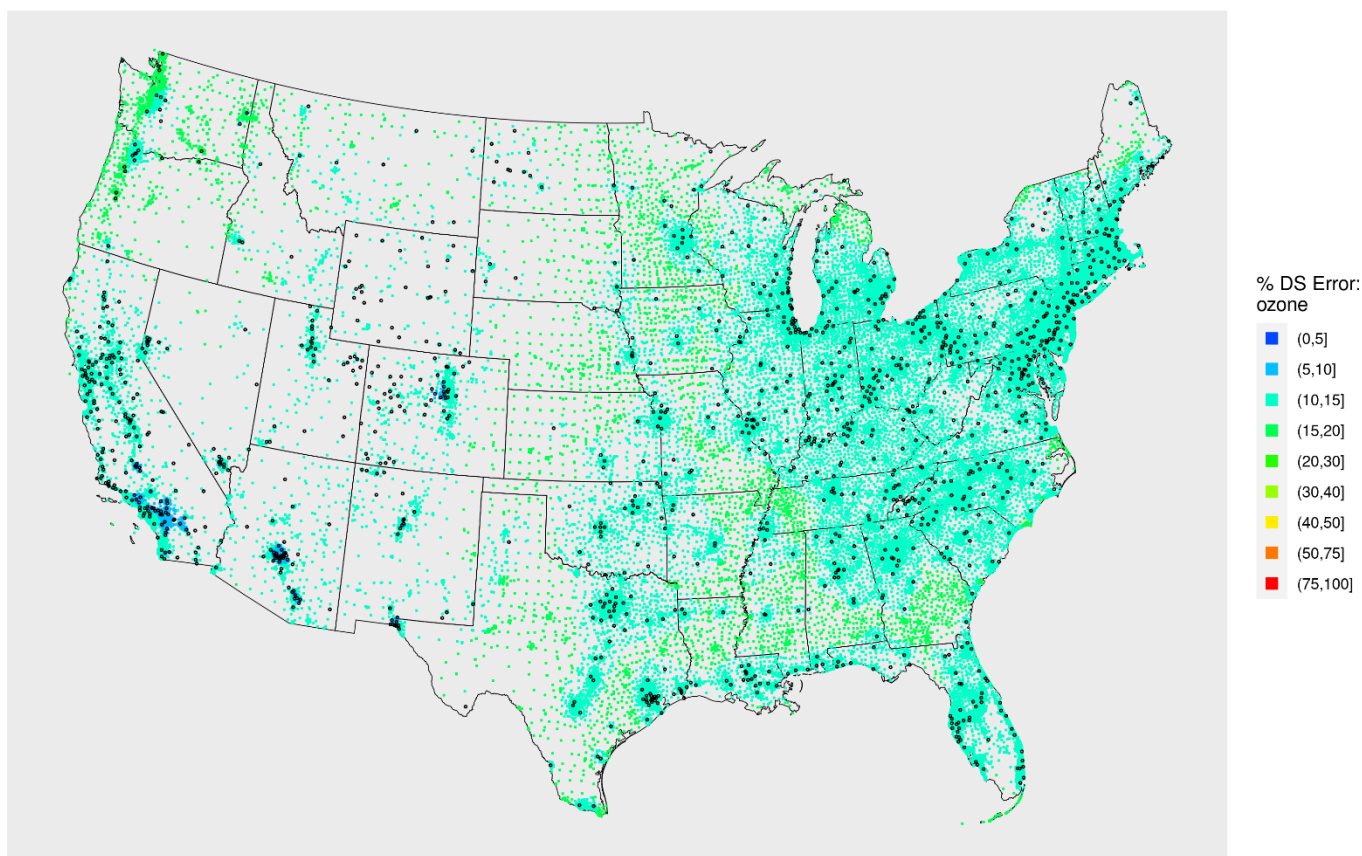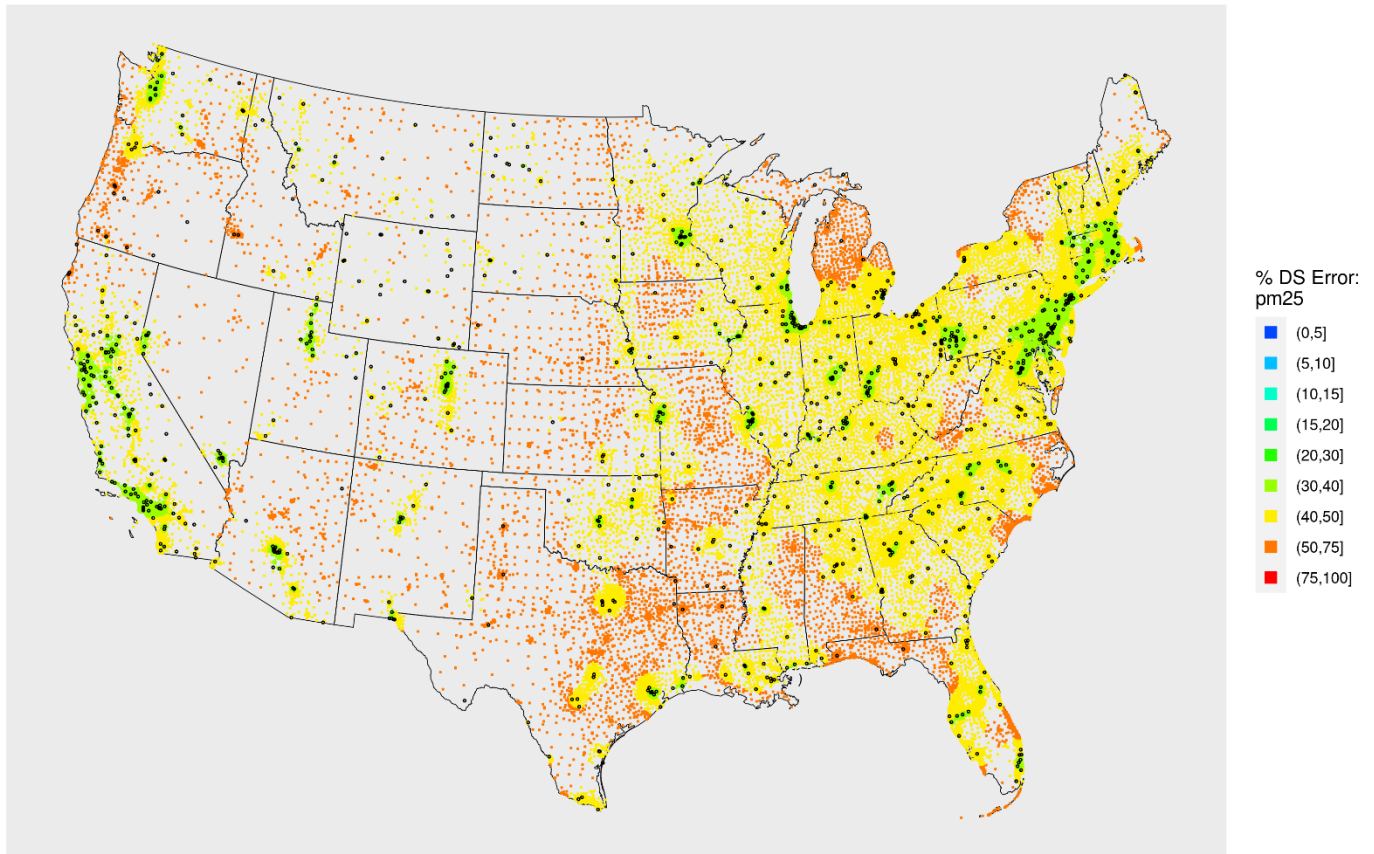
Figure 5-4. Annual mean relative errors (standard errors divided by predictions) from the DS 2018 runs. The black dots show the locations of monitors that generated the AQS data used as input to the DS model.

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
PM$_{2.5}$	973	0.19	3.54	0.95
O$_3$	1267	-0.01	4.36	0.95

Table 5-1. Cross-validation statistics associated with the 2018 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 2018. 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 grid cell. Care needs to be taken not to over-interpret any within-grid cell gradients that might be produced by a user. Fine-scale emission sources in CMAQ are diluted into the grid cell averages, but a given source within a grid cell 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 grid cell.

Appendix A - Acronyms

<u>Acronyms</u>

ARW	Advanced Research WRF core model
BEIS	Biogenic Emissions Inventory System
BlueSky	Emissions modeling framework
BSP	BlueSky Pipeline modeling system
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
HC	Hydrocarbon
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
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

Appendix B – Emissions Totals by Sector

Please see the independent spreadsheet AppendixB_2018_emissions_totals_by_sector.xlsx that provides inventory and speciation emissions totals for each emissions modeling sector.