LADCO | LAKE MICHIGAN AIR DIRECTORS CONSORTIUM

2022 Base Year and Analytic Year Air Quality Modeling Platform

Emissions and Air Quality Modeling Protocol

Lake Michigan Air Directors Consortium

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DOCUMENT CHANGE LOG

Version	Date	Comments/Changes
1	1/14/2025	Initial version for review by states and U.S. EPA
2	2/3/2025	Integrates comments on version 1

FIGURES

1 INTRODUCTION

The Lake Michigan Air Directors Consortium (LADCO) was established by the states of Illinois, Indiana, Michigan, and Wisconsin in 1989. The four states and U.S. EPA signed a Memorandum of Agreement (MOA) that initiated the Lake Michigan Ozone Study and identified LADCO as the organization to oversee the study. Additional MOAs were signed by the states in 1991 (to establish the Lake Michigan Ozone Control Program), January 2000 (to broaden LADCO's responsibilities), and June 2004 (to update LADCO's mission and reaffirm the commitment to regional planning). In March 2004, Ohio joined LADCO. Minnesota joined the Consortium in 2012. LADCO consists of a Board of Directors (i.e., the State Air Directors), a technical staff, and various workgroups. The main purposes of LADCO are to provide technical assessments for and assistance to its member states, and to provide a forum for its member states to discuss regional air quality issues.

LADCO will simulate air quality for a 2022 base year and multiple projection years to provide technical information in support of the LADCO states' Clean Air Act obligations to demonstrate and meet attainment of the National Ambient Air Quality Standard (NAAQS) for ozone (O_3) and fine particulate matter ($PM_{2.5}$). We anticipate that states may use the air quality simulations for attainment demonstration modeling, interstate transport modeling, and source-receptor culpability assessments.

LADCO will conduct the 2022 base year simulation using the regional air quality model Comprehensive Air Quality Model with Extensions (CAMx; Ramboll, 2024). After successful completion of the 2022 base year simulation, LADCO will simulate projected air pollution concentrations for the years 2026 and 2032. LADCO will use a two-way nested grid configuration with two modeling domains that zoom in on Lake Michigan. The outer 12-km domain will include the entire Continental US and parts of the Canada and Mexico. The inner 4-km domain will include all six LADCO states.

This document describes how LADCO will prepare emissions estimates for each of the modeling years and use CAMx to estimate air pollution concentrations in each year.

1.1 Air Quality Standards and Air Quality Related Values

The United State Environmental Protection Agency (U.S. EPA) sets National Ambient Air Quality Standards (NAAQS) for six regulated air quality pollutants: O_3, particulate matter (PM), sulfur dioxide (SO_2), nitrogen dioxide (NO_2), carbon monoxide (CO) and lead (Pb). After promulgation of a NAAQS, U.S. EPA designates nonattainment areas (NAAs) and states are required to submit State Implementation Plans (SIPs) to U.S. EPA that contain emission control plans and a demonstration that the NAA will achieve the NAAQS by the required date.

In 1997, U.S. EPA promulgated the first 8-hour O_3 NAAQS with a threshold of 0.08 ppm (84 ppb). On March 12, 2008, they promulgated a more stringent 0.075 ppm (75 ppb) 8-hour O_3 NAAQS. On October 1, 2015, U.S. EPA further strengthened the standard with the 0.070 ppm (70 ppb) 8-hour O_3 NAAQS. Figure 1-1 displays the locations of ozone nonattainment areas under the 2015 O_3 NAAQS.

On February 7, 2024, U.S. EPA revised the $PM_{2.5}$ primary NAAQS by lowering the annual $PM_{2.5}$ NAAQS threshold from 12.0 µg/m^3 to 9.0 µg/m^3; U.S. EPA retained the 24-hour $PM_{2.5}$ primary NAAQS at 35 µg/m^3. U.S. EPA also retained the 24-hour inhalable particles NAAQS (PM_{10}) at 150 µg/m^3. Figure 1-2 shows the locations of $PM_{2.5}$ nonattainment areas under the 2012 annual $PM_{2.5}$ NAAQS; final designations for the 2024 annual $PM_{2.5}$ NAAQS are not expected until January 2026.

In February 2010, U.S. EPA issued a new 1-hour NO_2 NAAQS with a threshold of 100 ppb. They have not yet designated nonattainment counties for the 1-hour standard. U.S. EPA promulgated an updated 1-hour SO_2 NAAQS in June 2010 with a threshold of 75 ppb. NAA designations for the SO_2 NAAQS began in October 2013, with subsequent rounds of designations continuing through April 2018. As of September 27, 2010, U.S. EPA has redesignated as maintenance areas all NAAs for Carbon Monoxide (CO). U.S. EPA issued a new lead NAAQS in 2008 and, except for Los Angeles, all the NAAs reside in the eastern or central U.S or Alaska. SO_2, CO, and lead are local NAAQS issues assessed on a local scale. Regional models assess ozone and fine particulate NAAQS issues because the precursors to these pollutants travel long distances. In this regional modeling protocol, we show only NAA designation maps for ozone and fine particulates.

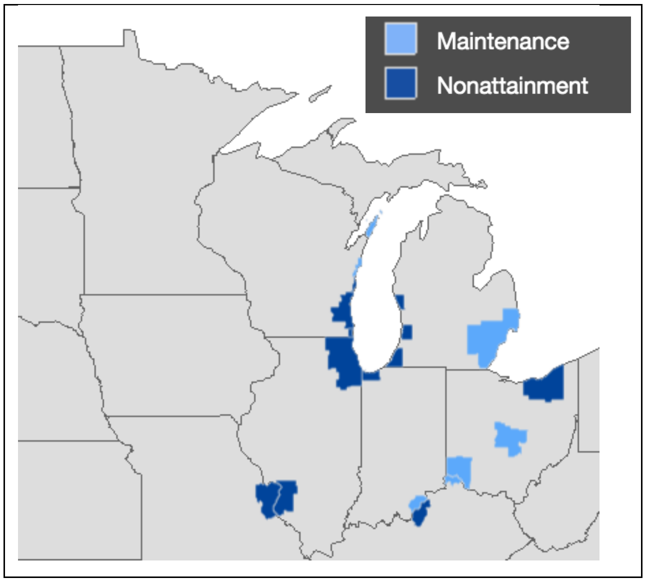

Figure 1-1. Current LADCO region ozone nonattainment and maintenance areas under the 2015 8-hour ozone NAAQS

Figure 1-2. Current LADCO nonattainment areas under the 2012 annual $PM_{2.5}$ NAAQS

1.2 Organization of the Modeling Protocol

This document presents the LADCO protocol for simulating emissions and air quality in the LADCO region for 2022, 2026, and 2032. The LADCO 2022 WRF model performance evaluation report (LADCO, 2024) documents the meteorology used in these simulations. The air quality modeling protocol is organized into the following sections:

1. Introduction: Summarizes the background, purpose and objectives of the study.
2. Model Selection: Describes the regional models selected for the study.
3. Episode Selection: Describes the modeling period for the study.
4. Modeling Domain Selection: Presents the modeling domains and grid structure for the modeling study.
5. WRF Meteorology: Describes how LADCO conducted the meteorological modeling and evaluated the WRF model simulation.
6. Emissions: Describes the emissions input data, how LADCO will conduct the emissions modeling, and the procedures for evaluating and validating the emissions processing results.
7. Photochemical Modeling: Describes the procedures for conducting the photochemical grid model including the model versions, inputs and options.
8. Model Performance Evaluation: Provides the procedures for conducting the model performance evaluation of the photochemical grid models.

9. Attainment Testing: Describes the model attainment test procedures for ozone and fine particulate matter
10. Documentation and Schedule: Describes how the project will be documented and the proposed schedule for modeling and documentation
11. References: Lists the references cited in the document.

1.3 Project Participants

Cooperators on the project include Federal agencies and state departments of environmental management. The LADCO Technical Oversight Committee (TOC) is composed of air quality modeling and planning branch staff in the LADCO member states. LADCO will interact with the TOC on the schedule, deliverables, and modeling results continually during this project. LADCO will also coordinate with federal agencies, including the U.S. EPA Office of Air Quality Planning and Standards and U.S. EPA Region 5, during this project. LADCO facilitates and manages the study and conducts an evaluation of the emissions and air quality modeling results. Key contacts and their roles in the LADCO 2022 emissions and air quality modeling are listed in Table 1-1.

Table 1-1. Key contacts for the LADCO 2022 emissions and air quality modeling platform

Name	Role	Organization/Contact
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Melissa Sheffer	EPA Region 5 Air Quality Modeling Advisor	U.S. EPA Region 5 Sheffer.Melissa@epa.gov

1.4 Related Studies

CAMx was used in several recent air quality modeling studies to simulate ozone formation in the LADCO region. We will apply some of the modeling approaches used in previous modeling studies to the new, 2022 base year and projection year modeling applications. These prior modeling efforts are described below. For all the studies described here, LADCO conducted the WRF, SMOKE, and air quality modeling used in the study, except where noted otherwise. LADCO provides the processed meteorology, emissions, and air quality data to our member states to support air quality planning and SIP analyses.

1.4.1 LADCO Attainment Demonstration Modeling for the 2015 Ozone NAAQS

LADCO (2022) used CAMx v7.10 to support the development of 2015 O_3 NAAQS NAA SIPs for the LADCO member states. The LADCO CAMx modeling results were used to identify O_3 monitoring sites that had nonattainment or maintenance problems for the 2015 O_3 NAAQS by the August 3, 2024 attainment date for moderate NAAs. LADCO used 2016 as the base modeling year from which we projected air quality in 2023. LADCO based our 2023 O_3 air quality and NAA attainment forecasts on meteorology modeling that was optimized for conditions in the Great Lakes Basin. We used U.S. EPA 2016fh emissions modeling platform data, and other CAMx modeling platform inputs released by the U.S. EPA in September 2019 as inputs to this modeling application. LADCO replaced the Electricity Generating Unit (EGU) emissions in the 2016fh platform with 2023 EGU forecasts estimated with the ERTAC EGU Tool version 22V1. ERTAC EGU 22V1 integrated state-reported information on EGU operations and forecasts as of September 2021.

1.4.2 LADCO Attainment Demonstration Modeling for the 2008 Ozone NAAQS

LADCO (2020) used CAMx v7.0 to support the development of the O_3 NAA SIPs for the states of Wisconsin, Illinois, and Indiana pursuant to the 2008 O_3 NAAQS. LADCO used 2016 as the base modeling year from which we projected air quality in 2020. LADCO based the 2020 ozone air quality and NAA attainment forecasts on the CAMx modeling platform released by the U.S. EPA in September 2019 to support regional haze progress assessments. LADCO adapted the U.S. EPA regional haze platform to estimate ozone design values. LADCO estimated 2020 emissions for most of the anthropogenic inventory sectors by interpolating between the 2016 and 2023 National Emissions Collaborative (NEC) 2016v1 inventories. We used linear interpolation for the emissions because 2020 inventories were not readily available for all sectors at the time that this application initiated. LADCO replaced the Electricity Generating Unit (EGU) emissions in the U.S. EPA 2016fh_16j platform with 2020 EGU forecasts estimated with the ERTAC EGU Tool version 16.1.

1.4.3 LADCO 2015 Ozone NAAQS Good Neighbor SIP Modeling

LADCO (2018a) conducted CAMx modeling in the spring/summer of 2018 to support the 2015 Ozone NAAQS “Good Neighbor” SIPs for the LADCO states. LADCO adapted the U.S. EPA 2011 “EN” modeling platform, which included projections to 2023, for simulating the impacts of emissions controls on ground level O_3. CAMx source apportionment modeling with the Anthropogenic Precursor Culpability Assessment (APCA) tool was used to quantify emissions source region and sector impacts on O_3 concentrations at downwind receptors. LADCO modified the U.S. 2023EN inventory by replacing the U.S. EPA electricity generating unit projections with the Eastern Regional Technical Advisory Committee (ERTAC) EGU projections for power sector sources. LADCO used the CAMx modeling results to develop future year O_3 design values. LADCO also used the results to quantify the impact of source regions and inventory sectors on the design values.

1.4.4 LADCO Modeling and Analysis for Demonstrating Reasonable Progress for the Regional Haze Rule 2018 - 2028 Planning Period

LADCO (2021) prepared this Technical Support Document to support the development of regional haze state implementation plans (SIPs) for the second haze implementation period. We used the CAMx version 7.10 regional air quality model to estimate 2011 and 2016 base years and 2028 future year PM concentrations and haze conditions. LADCO relied upon U.S. EPA's inventory estimates from their 2011 and 2016 modeling platforms for most emissions sectors. However, LADCO replaced the Integrated Planning Model (IPM) EGU inventories in the U.S. EPA 2011 and 2016 modeling platforms with inventories derived from the Eastern Regional Technical Advisory Committee (ERTAC) EGU model (MARAMA, 2012). We configured CAMx with the Particulate Matter Source Apportionment Tool (PSAT) to calculate emissions tracers for identifying upwind sources of haze at downwind Class I areas. Overall, this document describes how LADCO used CAMx modeling to simulate base and future year air quality, and to evaluate if the Class I areas in and near the LADCO region are projected to meet or exceed the uniform rate of progress toward natural visibility conditions in 2064. The CAMx modeling outputs of this work were provided to the LADCO state air programs to support their RHR SIP revisions.

LADCO will apply many of the same modeling approaches used in these studies for the 2022 modeling described in this protocol. The SMOKE processing approaches, the CAMx modeling configuration, and the CAMx data post-processing and analysis used in these studies will be adapted for the 2022 modeling described in this protocol.

1.5 Overview of LADCO 2022 Modeling Approach

The procedures for the LADCO 2022-based modeling will generally follow our approach used for the 2015 O_3 NAAQS Transport modeling (LADCO, 2022). LADCO will adapt the U.S. EPA 2022hc emissions modeling platform to create a LADCO 2022 modeling platform. The LADCO 2022 modeling platform will include 12 km and 4 km modeling domains that focus on the LADCO region. The LADCO 4 km domain was designed to encompass the entirety of the LADCO region. LADCO will project the 2022 emissions to various future years to test attainment of the O_3 and $PM_{2.5}$ NAAQS, and to perform targeted emissions sensitivity tests. The LADCO 2022 modeling approach is summarized below, with more details provided in the chapters of this modeling protocol.

- The modeling period will encompass the 2022 calendar year with a 10-day spin-up period at the end of 2021.
- Year 2022, 2026, and 2032 inventories will be used to estimate base and future year emissions for the LADCO states.
- A 12 km continental U.S. (CONUS; 12US2) domain and 4 km LADCO region (LADCO4) domain will be simulated using CAMx.
- Year 2022 Weather Research Forecasting (WRF) modeling results generated by LADCO (2024a,b) will be used to provide meteorology inputs for the LADCO 2022 modeling platform.

- Emissions modeling will be primarily conducted using the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system using mainly emissions data from the NEC 2022v1 platform.
- The ERTAC EGU model will be used to forecast emissions for electricity generating unit sources.
- Photochemical grid modeling is based on the Comprehensive Air-quality Model with extensions (CAMx) version 7.31 (Emery et al., 2024). The Carbon Bond 7 revision 1 (CB7r1) gas phase chemistry, ISORROPIA inorganic gas-aerosol partitioning, SOAP3 organic gas-aerosol partitioning and oxidation, and static Coarse and Fine mode (CF) particle size distribution. In the CAMx simulation, gaseous and aerosol chemistry is calculated using a source file of 'CAMx7.3.chemparam.CB7r1_CF3_COMPLX'.
- Hourly boundary conditions (BCs) for the lateral boundaries of the 12--km CONUS domain will be taken from U.S. EPA 2022 Hemispheric CMAQ modeling[1].
- Model evaluation will be conducted for O_3 and fine particulate matter ($PM_{2.5}$) species using published model performance metrics.

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[1] Accessed January 2025 from https://registry.opendata.aws/epa-2022-modeling-platform

2 MODEL SELECTION

This section discusses the modeling software that LADCO will use for the 2022 modeling platform. The selection methodology for modeling software follows U.S. EPA's guidance for regulatory modeling in support of O_3 and $PM_{2.5}$ air quality goals (U.S. EPA, 2018a). U.S. EPA recommends that models be selected for regulatory O_3, PM and visibility studies on a "case-by-case" basis with appropriate consideration being given to the candidate models':

- Technical formulation, capabilities and features;
- Pertinent peer-review and performance evaluation history;
- Public availability; and
- Demonstrated success in similar regulatory applications.

All these considerations should be examined for each class of models to be used (e.g., emissions, meteorological, and photochemical) in part because U.S. EPA no longer recommends a specific model or suite of photochemical models for regulatory application as it did twenty years ago in the first O_3 SIP modeling guidance (U.S. EPA, 1991). Below are the candidate models we believe are best suited to the requirements of the LADCO region. Included are the candidate model attributes and justification for the models selected using the four criteria above. The science configurations recommended for each model in this study are introduced in Chapter 5**.**

2.1 Justification and Overview of Selected Models

LADCO will use three general types of models to simulate O_3, and other gaseous pollutants, particulate matter, visibility, and deposition:

- Meteorological Models (MM)
- Emissions Models (EM)
- Photochemical Grid Models (PGM)

These are not single pieces of software, but rather software suites that are used to generate PGM meteorological and emissions inputs and simulate air quality, visibility and deposition.

2.1.1 Meteorological Model

The Weather Research Forecast (WRF) model is currently the only prognostic meteorological model that is routinely used in the U.S. in photochemical grid modeling studies. WRF was developed by the regional climate modeling community with support and coordination provided by the National Center for Atmospheric Research (NCAR). LADCO is using 2022 meteorology fields that we simulated using WRF Version 4.5 for the 12-km grid resolution domain covers the continuous U.S. and the 4-km gid resolution domain expands over the Midwest. Based on following four selection criteria, WRF was selected as the meteorological model for the following reasons:

- Technical: WRF is based on recent physics and computing techniques. WRF is continuously updated with new capabilities and features and is actively supported by NCAR.

- Performance: WRF is being used by thousands of users and been subjected to a community peer-reviewed development process using the latest algorithms and physics. WRF has a rich publication and application history.
- Public Availability: WRF is publicly available and can be downloaded from the WRF website with no costs or restrictions.
- Demonstrated Success: LADCO WRF 2022 simulation (LADCO 2024a) has the lowest errors and biases for key surface meteorological variables in the Midwest for all seasons as compared to the USEPA's WRF 2022 modeling (USEPA 2024a). The 2017 Lake Michigan Ozone Study (Pierce et al., 2018) showed that when properly configured, WRF is the best model for simulating high O_3 events on the Lake Michigan shoreline. The U.S. EPA (2018b) demonstrated acceptable WRF performance for retrospectively simulating 2016 meteorology, particularly for use in air quality modeling.

More details on the selected WRF meteorological model are provided below.

WRF: The non-hydrostatic version of the Advanced Research version of the Weather Research Forecast (WRF-ARW[2]) model (Skamarock et al. 2004; 2005; 2006; Michalakes et al. 1998; 2001; 2004) is a three-dimensional, limited-area, primitive equation, prognostic model that has been used widely in regional air quality modeling applications. The basic model has been under continuous development, improvement, testing and open peer-review for nearly 20 years and has been used world-wide by hundreds of scientists for a variety of mesoscale retrospective and forecasting applications. WRF is a next-generation mesoscale prognostic meteorological model routinely used for urban- and regional-scale photochemical, fine particulate and regional haze regulatory modeling studies. Developed jointly by NCAR and the National Centers for Environmental Prediction, WRF is maintained and supported as a community model by researchers and practitioners around the world. The code supports two modes: the Advanced Research WRF (ARW) version and the Non-hydrostatic Mesoscale Model (NMM) version. WRF-ARW is the standard regional climate model for regulatory air quality applications in the U.S. It is suitable for use in a broad spectrum of applications across scales ranging from hundreds of meters to thousands of kilometers.

2.1.2 Emissions Processing Systems

Emissions data for PGMs are prepared with a suite of data processing and modeling software. The basic component of the emissions modeling software suite is a processor to convert emission inventory data into PGM input files. Additional emissions modeling software target specific emissions sectors, including biogenic sources, on-road mobile sources, windblown dust, lightning, and sea spray. The emissions processors are routinely used in the U.S. in photochemical grid modeling studies:

- The Emissions Modeling System (EMS); and
- The Sparse Matrix Operator Kernel Emissions (SMOKE) system.

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[2] All references to WRF in this document refer to the WRF-ARW

EMS and SMOKE are emissions processors, not emissions models. The primary function of these tools is to convert emission inventory data to the spatial, chemical, and temporal terms required by a particular PGM.

Based on the four selection criteria, we will use the SMOKE system for the LADCO 2022 air quality simulation for the following reasons:

- Technical: Of the two emissions processors listed above, SMOKE is undergoing the most active development. Updates to SMOKE occur at least annually to add new capabilities and features and to address bugs and inefficiencies. SMOKE is widely used for regulatory modeling studies and is the only emissions processor in use by U.S. EPA.
- Performance: SMOKE is designed to be efficient in how it processes large quantities of data.
- Public Availability: SMOKE is publicly available for download from the Community Modeling and Analysis System (CMAS) Center with no costs or restrictions.
- Demonstrated Success: All regional air quality modeling studies in the last five years outside of California and Texas used SMOKE to prepare the emissions data. SMOKE has proven to be a reliable system for processing the data into the gridded hourly and chemically speciated emission inputs needed for PGM modeling.

SMOKE is a set of programs that is used by the U.S. EPA, MJOs, and state environmental agencies to prepare emissions inventory data for input to PGMs. SMOKE converts annual, daily, or hourly estimates of emissions at the state or county level to hourly emissions fluxes on a uniform spatial grid that are formatted for input to either the CMAQ or CAMx PGMs. SMOKE integrates county-level emissions inventories with source-based temporal, spatial, and chemical allocation profiles to create hourly emissions fluxes on a predefined model grid. For elevated sources that require allocation of the emissions to the vertical model layers, SMOKE integrates meteorology data to derive dynamic vertical profiles. In addition to its capacity to simulate emissions from stationary area, stationary point, and on-road mobile sectors, SMOKE is also instrumented with the Biogenic Emissions Inventory System, version 3 (BEIS3) model for estimating biogenic emissions fluxes (Vukovich and Pierce, 2002). The SMOKE-MOVES processor is an interface for the MOVES on-road mobile emissions model that prepares MOVES results for input to a PGM. SMOKE also can calculate future-year emissions estimates, if the user provides data about how the emissions will change in the future.

SMOKE uses C-Shell scripts as user interfaces to set configuration options and call executables. SMOKE has flexible QA capabilities to generate standard and custom reports for checking the emissions modeling process. The efficient processing of SMOKE makes it an appropriate choice for handling the large processing needs of regional and seasonal emissions processing, as described in more detail by Houyoux et al. (1996, 2000).

SMOKE is a software tool and not a set of data files; therefore, SMOKE relies on user-provided data files for emission inventories and factors to apply to those emissions. The emission factors assign the annual inventory data to the hours, grid cells, and model species and can be adjusted by the user in a way that is the most appropriate for the inventory sources included in the air quality modeling domain. In addition, SMOKE requires meteorology data in the Input/Output Application Programmers Interface (I/O API) format to process meteorology-dependent emissions sectors. The input meteorology dictates the temporal and spatial extents of the SMOKE modeling periods. SMOKE can neither interpolate between different grid resolutions nor project/backcast to dates that are not covered in the input meteorology. SMOKE has strict requirements for the nature and formats of the inventory data that it can use.

SMOKE primarily uses two types of input file formats: ASCII files and I/O API netCDF files. Input files are files read by at least one core SMOKE program but are not written by a core program. SMOKE uses strict rules that define the format and content of the input files. All data input to SMOKE must be either formatted to one of the prescribed input file types or converted to an intermediate form, such as a gridded I/O API inventory file, before it can be input to SMOKE.

SMOKE requires an emissions inventory, temporal allocation, spatial allocation, and chemical allocation data to prepare emissions estimates for an air quality model. For some source categories, such as on-road mobile and stationary point sources, SMOKE also requires meteorology data to calculate emissions. SMOKE calculates biogenic emissions estimates with gridded land use, vegetative emissions factors, and meteorology data.

Upstream software and utilities are used to prepare many of the inputs to SMOKE. The Meteorology Chemistry Interface Processor (MCIP), part of the Community Multiscale Air Quality (CMAQ) model, is used to prepare WRF meteorology data for input to SMOKE. A Geographic Information System (GIS), such as the open-source Spatial Allocator, creates the spatial surrogates that map inventory data to modeling grids. The Speciation Tool is built on top of the SPECIATE database as an interface to create the chemical allocation profiles that convert inventory pollutants to PGM species. Temporal allocation profiles and the assignment files that associate the spatial/chemical/temporal profiles to inventory sources are all available through an ad-hoc database from the U.S. EPA Clearinghouse for Inventories and Emissions Factors. Other source-specific inputs, such as land use/land cover data for biogenic emissions and Motor Vehicle Emissions Simulator (MOVES) look up tables and ancillary files, are typically prepared for SMOKE on a project-specific basis. The next section provides details on the data use for this study.

MOVES: The MOtor Vehicle Emission Simulator model (MOVES) is a multi-scale emissions modeling system that generates emission inventories or emission rate lookup tables for on-road and off-road mobile sources. The EPA's Office of Transportation and Air Quality (OTAQ) designed MOVES.

For the on-road sector, MOVES can create inventories or lookup tables at the national, state, county, or project scales. MOVES is principally an emissions modeling system where emissions estimates are simulated from 'first principles' and take into account the effects of fleet age deterioration, ambient temperature and humidity, activity patterns, fuel properties, and inspection and maintenance programs on emissions from all types of motor vehicles.

For the off-road sector, MOVES creates inventories on the national or county scale. MOVES version 4 (MOVES4), released in August 2023, was available at the time of the development of the LADCO2022v1 modeling. MOVES4 provides significant improvements to emission estimates over previous versions.

MOVES outputs can be input to emissions processing systems such as SMOKE for both the on-road and off-road sectors.

2.1.3 Photochemical Grid Model

There are two PGMs that are widely used for O_3, $PM_{2.5}$ and visibility planning in the U.S.:

- Community Multiscale Air Quality (CMAQ) modeling system developed by U.S. EPA; and
- Comprehensive Air-quality Model with extensions (CAMx) developed by Ramboll.

Both models are publicly available and have adopted the "one-atmosphere" concept treating O_3, $PM_{2.5}$, air toxics, visibility and other air quality issues within a single platform.

- Technical: Both CMAQ and CAMx have adopted the state-of-science "one-atmosphere" concept for treating O_3, $PM_{2.5}$, air toxics and other air quality issues within a single platform. We selected CAMx for the LADCO 2022 air quality simulation because the model supports two-way grid nesting and source apportionment techniques.
- Performance: Both CMAQ and CAMx perform similarly when compared to ambient surface observations.
- Public Availability: CMAQ and CAMx are both publicly available.
- Demonstrated Success: Both CMAQ and CAMx have had many successful model performance applications.

The CAMx and CMAQ models are summarized below.

CAMx: The Comprehensive Air Quality Model with Extensions modeling system is a state-of-science 'One-Atmosphere' photochemical grid model capable of addressing Ozone, particulate matter (PM), visibility and acid deposition at regional scale for periods up to one year (Ramboll, 2024). CAMx is a publicly available open-source computer modeling system for the integrated assessment of gaseous and particulate air pollution. Built on today's understanding that air quality issues are complex, interrelated, and reach beyond the urban scale, CAMx is designed to (a) simulate air quality over many geographic scales, (b) treat a wide variety of inert and chemically active pollutants including O_3, inorganic and organic $PM_{2.5}$ and PM_{10} and mercury and toxics, (c) provide source-receptor, sensitivity, and process analyses, and (d) be computationally efficient and easy to use.

U.S. EPA has approved the use of CAMx for numerous O_3 and PM State Implementation Plans throughout the U.S. and U.S. EPA has used CAMx to evaluate regional mitigation strategies including those for recent regional rules (e.g., CSAPR, CATR, CAIR, NO_X SIP Call, etc.).

CMAQ: U.S. EPA's Models-3/Community Multiscale Air Quality (CMAQ) modeling system is also a "one-atmosphere" photochemical grid model capable of addressing O_3, PM, visibility and acid deposition at regional scale for periods up to one year. The CMAQ modeling system was designed to approach air quality by including state-of-the-science capabilities for modeling multiple air quality issues, including tropospheric O_3, fine particles, toxics, acid deposition, and visibility degradation. CMAQ was also designed to have multi-scale capabilities so that separate models were not needed for urban and regional scale air quality modeling.

LADCO selected CAMx for this study because it is a component of recent LADCO, state, and U.S. EPA modeling platforms for investigating and demonstrating attainment of the NAAQS (LADCO 2017; LADCO, 2020; LADCO, 2022), and for quantifying the relationships between emissions sources and receptors (LADCO, 2018; LADCO 2021; U.S. EPA 2016). As CAMx is a component of U.S. EPA studies with a similar scope to this project, LADCO can leverage the data and software elements that are distributed with U.S. EPA regulatory modeling platforms. Using these elements saves LADCO significant resources relative to building a modeling platform from scratch. The CAMx source apportionment capabilities will allow LADCO to investigate the sources of air pollution impacting surface air quality monitors within and downwind of the LADCO region.

The WRF meteorological model Version 4.5 (April 20, 2023) was applied to the 2022 modeling episode and grid structure. LADCO will use the WRFCAMx version 5.2 program to generate meteorological inputs for the CAMx model from WRF output.

LADCO intends to use Boundary Conditions (BCs) for the 12 km CONUS domain based on output from a hemispheric application of CMAQ developed by U.S. EPA. Alternative sources of BCs, such as the GEOS-Chem Global Chemistry Model (GCM) may also be considered.

3 EPISODE SELECTION

EPA’s O_3, $PM_{2.5}$ and visibility modeling guidance (U.S. EPA, 2018a) contains recommended procedures for selecting modeling episodes. Per this guidance, this chapter presents the justification for selecting 2022 for the modeling period.

3.1 Episode Selection Criteria

The U.S. EPA modeling guidance lists primary criteria for selecting episodes for O_3 and $PM_{2.5}$ SIP modeling along with a set of secondary criteria to consider.

3.1.1 Primary Episode Selection Criteria

The U.S. EPA modeling guidance (US EPA, 2018a) identifies four specific criteria to consider when selecting episodes for use in demonstrating attainment of the 8-hour O_3 or $PM_{2.5}$ NAAQS:

1. A variety of meteorological conditions should be covered, including the types of meteorological conditions that produce O_3 and $PM_{2.5}$ exceedances in LADCO region;
2. Choose time periods with observed concentrations that are close to O_3 and $PM_{2.5}$ Design Values, or to the level of visibility impairment such that relative response factors (RRFs) can be based on several (i.e., > 10) days with at least 5 days being the absolute minimum;
3. To the extent possible, the modeling period should include days for which extensive databases (i.e. beyond routine aerometric and emissions monitoring) are available; and
4. Variability in the observed pollution concentrations across the period to ensure that the model characterizes high and low pollution conditions and demonstrates skill in simulating the transition periods between pollution episodes .

3.1.2 Secondary Criteria

U.S. EPA also lists four “other considerations” to bear in mind when choosing potential 8-hour O_3 or $PM_{2.5}$ episodes, including:

1. Choose periods which have already been modeled;
2. Choose periods that are drawn from the years upon which the current Design Values are based;
3. Include weekend days among those chosen; and
4. Choose modeling periods that meet as many episode selection criteria as possible in the maximum number of nonattainment areas as possible.

U.S. EPA suggests that modeling an entire summer O_3 season for O_3 or an entire year for $PM_{2.5}$ would be a good way to assure that a variety of meteorological conditions are captured and that sufficient days are available to construct robust relative response factors (RRFs) for the 8-hour O_3 and $PM_{2.5}$ Design Value projections.

3.2 Episode Selection Results

LADCO selected the 2022 calendar year for modeling because it satisfied several of the episode selection criteria listed above than other recent years:

1. Modeling the entire year of 2022 will capture a variety of conditions that lead to elevated O_3 and $PM_{2.5}$ concentrations in the region
2. The NEC is creating 2022-base emissions (2022 Inventory Collaborative Wiki)
3. An annual simulation will assure sufficient days are available to analyze O_3 and $PM_{2.5}$ impacts. Annual simulations also allow the assessment of annual AQ/AQRV issues such as sulfur and nitrogen deposition, annual average NAAQS and annual average evaluation using NADP, CASTNet and other observation networks.
4. With an annual run, all weekend days in a year are included.

In 2023 the U.S. NEC held a series of phone meetings to identify a new base year to use for developing O_3, $PM_{2.5}$, and regional haze State Implementation Plans (SIPs). The collaborative process between the U.S. EPA, states, and Multi-Jurisdictional Organizations (MJOs), identified 2022 as the single most representative year in the range of years evaluated (2019-2022). LADCO selected 2022 as the base modeling year for this study because it is a recent year, and it included an O_3 season representative of recent conditions in the region.

Figure 3-1 shows that 2022 was an average year for maximum temperatures in the region compared to the 30-year average. Both 2021-and 2023 were warmer than average over the northern and western part of the domain, respectively. Figure 3-2 shows that relative to the O_3 design value trends since 2001, the average O_3 concentrations across the LADCO region increased through the period 2020-2022, which reflects a return to more typical air quality following the economic and societal upsets from the COVID-19 pandemic that peaked in 2020. The $PM_{2.5}$ design value trend shown in Figure 3-3 also demonstrates that 2022 was representative of recent years for fine particles. Data availability is also an important consideration in the selection of 2022 as a base modeling year.

Because the NEC recommended 2022 as the next national modeling base year after 2016, there are several readily available options for regional air quality modeling input data. The U.S. EPA has produced lateral boundary conditions, emissions, and meteorology data for 2022. The NEC developed (or will develop) 2022, 2026, and 2032 emissions modeling platforms to support air quality modeling over the Continental U.S.

Although a 2022 air quality modeling platform only has limited performance evaluation results[3], LADCO recommends 2022 as the base year because we will benefit from the multiple efforts at the U.S. EPA, states, and MJOs that are occurring in parallel to simulate and evaluate 2022 air quality. The decision to model the entire calendar year rather than just the summer O_3 season is due to a need to address $PM_{2.5}$ NAAQS issues.

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[3] See: https://gaftp.epa.gov/Air/aqmg/jhuang/2022modeling_platform/2024_Oct_FedState_Call_20241025_cleaned%20version.pptx

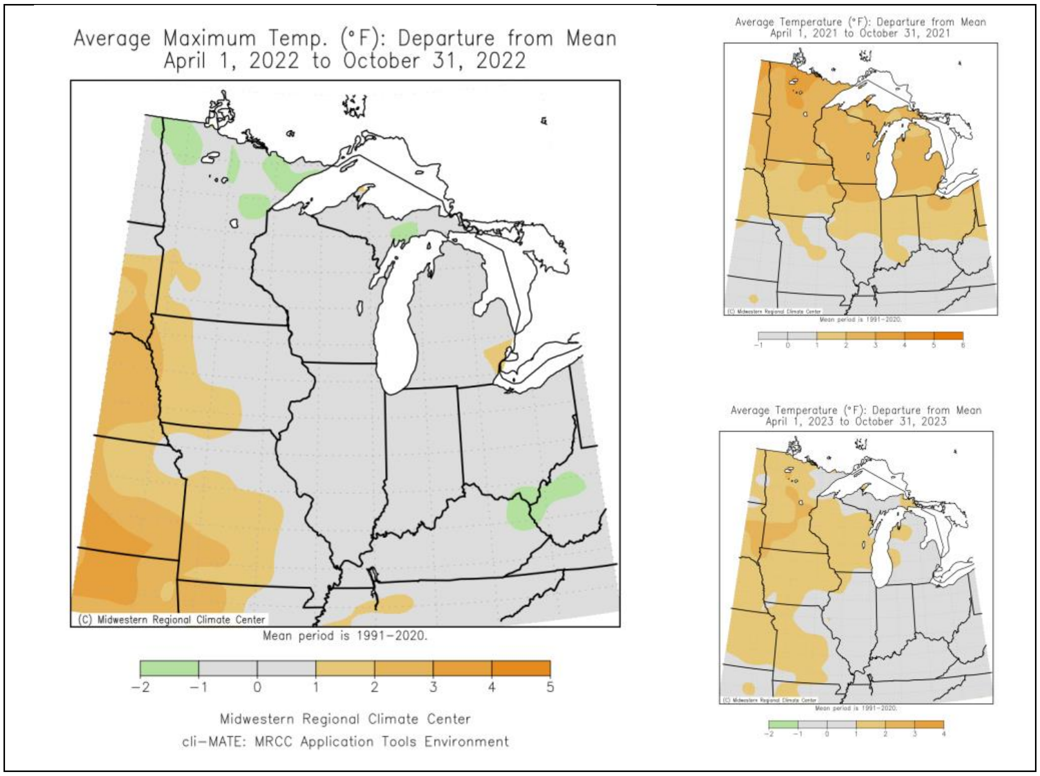

Figure 3-1. Midwest region 2021, 2022, and 2023 ozone season (Apr – Oct) temperature anomalies (Credit: Midwest Regional Climate Center).

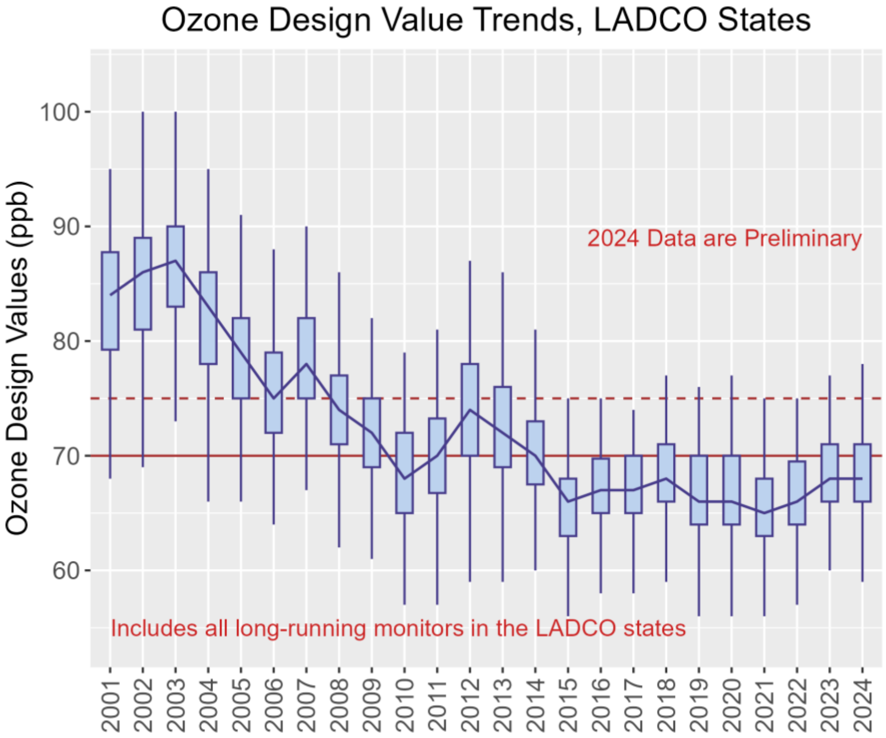

Figure 3-2. 3-year ozone design values at LADCO monitors; horizontal lines represent the 2008 and 2015 ozone NAAQS.

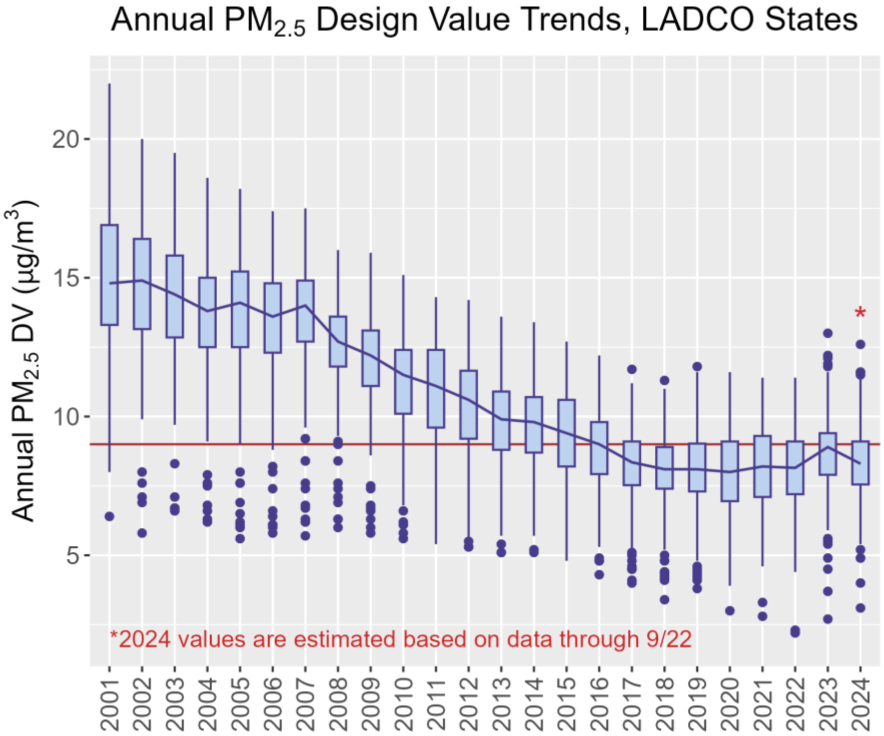

Figure 3-3. 3-year $PM_{2.5}$ design values at LADCO monitors; the horizontal line represents the 2024 annual $PM_{2.5}$ NAAQS.

4 DOMAIN SELECTION

This chapter summarizes the model domain definitions for the LADCO photochemical grid modeling (PGM), including the domain coverage, resolution, map projection, and nesting schemes for the 4-km sub-domain. The modeling domains for the WRF meteorological modeling are defined slightly larger than the PGM domains and are shown in Chapter 5. More details are in the LADCO WRF Modeling Protocol and Model Performance Evaluation Report (LADCO, 2024a and 2024b).

4.1 Horizontal Modeling Domain

The LADCO 2022 modeling domains were selected as a trade-off between the need to have high resolution modeling for receptors near the Lake Michigan shoreline and the ability to perform timely regional O_3 and $PM_{2.5}$ modeling for the LADCO states. The LADCO 2022 modeling will use continental 12-km and regional 4-km modeling domains. A Lambert Conformal Conic map projection (LCP) will be used for the LADCO 12/4 km horizontal modeling domains using the parameters in Table 4-1 with their extent illustrated in Figure 4-1**.**

- A 12 km contiguous U.S. (12US2) domain that is the same as used by the U.S. EPA. The domain is large enough to ensure the outer boundaries of the domain are far away from our primary areas of interest (i.e., LADCO states).
- A 4 km LADCO (LADCO4) domain contains all the LADCO states

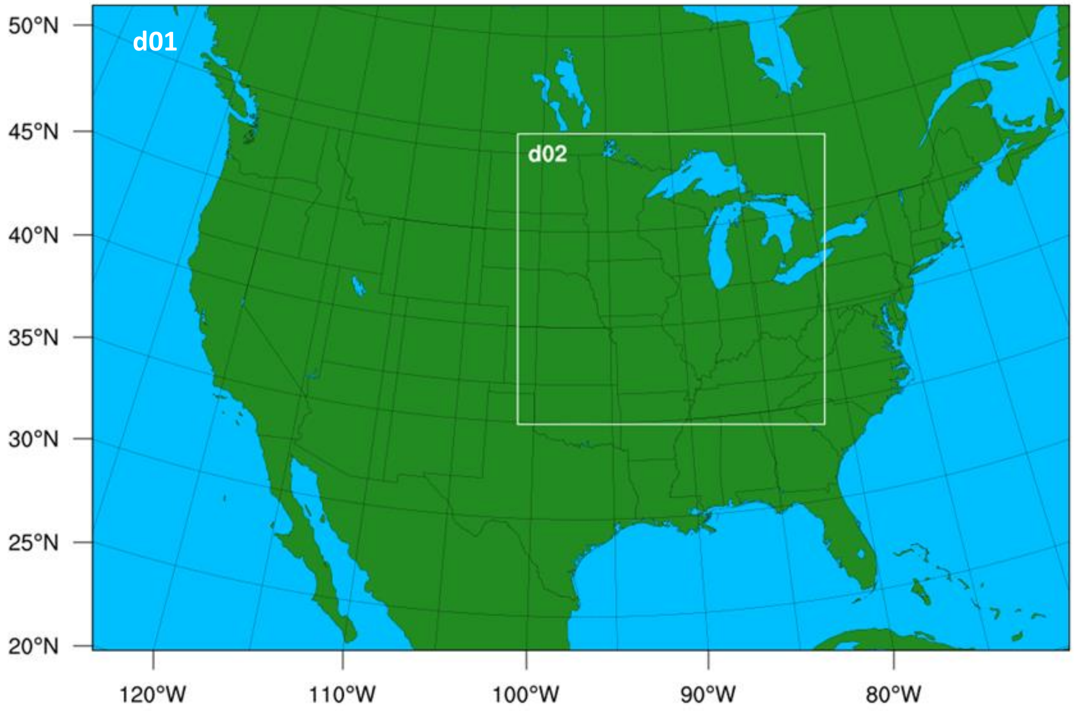

Figure 4-1. LADCO 12-km (d01) and 4-km (d02) CAMx modeling domains

Table 4-1. LADCO 2022 modeling domain configuration

Parameter	Value	
Projection	Lambert-Conformal	
1st True Latitude	33 degrees N	
2nd True Latitude	45 degrees N	
Central Longitude	-97 degrees W	
Central Latitude	40 degrees N	
Grid	D01 (12-km CONUS)	D02 (4-km Midwest)
Resolution (km)	12	4
Columns, Rows	396, 246	420, 390
X-origin, Y-origin (km)	-2412, -1620	-132, -420

4.2 Vertical Domain Structure

The CAMx vertical layer structure depends on the WRF vertical layer structure. The LADCO WRF 2022 simulation has 36 vertical layer interfaces (35 vertical layers using CAMx definition of layer thicknesses) from the surface up to 50 mb (LADCO, 2024a). The WRF model employs a terrain following coordinate system defined by pressure, using multiple layers that extend from the surface to approximately 19 km above mean sea level. We will retain all vertical WRF layers for the CAMx air quality simulations. Table 4-2 shows the vertical layer structure that LADCO will use to simulate 2022 air quality with CAMx.

Table 4-2. CAMx vertical layer structure

WRF Layer	Height (m)	Pressure (Pa)	Sigma	Thickness (m)
36	17,556	5000	0.000	2776
35	14,780	9750	0.050	1958
34	12,822	14500	0.100	1540
33	11,282	19250	0.150	1280
32	10,002	24000	0.200	1101
31	8,901	28750	0.250	969
30	7,932	33500	0.300	868
29	7,064	38250	0.350	789
28	6,275	43000	0.400	722
27	5,553	47750	0.450	668
26	4,885	52500	0.500	621
25	4,264	57250	0.550	581
24	3,683	62000	0.600	547
23	3,136	66750	0.650	517
22	2,619	71500	0.700	393
21	2,226	75300	0.740	285
20	1,941	78150	0.770	276
19	1,665	81000	0.800	180

18	1,485	82900	0.820	177
17	1,308	84800	0.840	174
16	1,134	86700	0.860	170
15	964	88600	0.880	167
14	797	90500	0.900	83
13	714	91450	0.910	82
12	632	92400	0.920	81
11	551	93350	0.930	81
10	470	94300	0.940	80
9	390	95250	0.950	79
8	311	96200	0.960	79
7	232	97150	0.970	78
6	154	98100	0.980	39
5	115	98575	0.985	38
4	77	99050	0.990	39
3	38	99525	0.995	19
2	19	99763	0.9975	19
1	0	100000	1.000	0

5 METEOROLOGICAL MODELING

This section describes the modeling software and approach that used for the 2022 WRF simulation. LADCO simulated the WRF meteorological model for the 2022 calendar year using a 12/4/1.33-km domain structure. We evaluated the WRF modeling results for the 2022 annual period against surface meteorological observations of wind speed, wind direction, temperature and humidity for each domain and compiled model performance statistics on seasonal and monthly basis. We compared the 2022-WRF model performance against meteorological modeling benchmarks and with previous meteorological model performances in the region (LADCO 2018; Brown, 2014; USEPA 2016; USEPA 2014). Although LADCO does not plan to run CAMx at 1.33-km for ozone or $PM_{2.5}$ attainment testing, we simulated a 1.33-km WRF domain to provide an option for air quality modeling at this resolution.

5.1 Model Selection and Application

LADCO used WRF version 4.5 to simulate meteorology in 2022. We will use the WRF preprocessor programs GEOGRID, UNGRIB, and METGRID to develop model inputs.

5.2 Topographic Inputs

Topographic information for the WRF was developed using the National Land Cover Database (NLCD) 2011 Update available from the National Center for Atmospheric Research (NCAR) based on the 30 sec (~1000 m) data for 12km domain and 9 sec (~300 m) data for finer domains, respectively[4]. More recent NLCD data formatted for input to WRF were not available at the time we started the LADCO WRF runs.

5.3 Vegetation Type and Land Use Inputs

We used 2011 National Landcover Data (NLCD) for the vegetation and land use inputs to WRF. The NLCD is a 40-category, 30-meter resolution dataset of land-cover for the continental U.S. We supplemented the WRF-compatible version of the NLCD with MODIS 20-category land cover data for regions outside of the U.S.

Table 5-1 lists the NLCD and MODIS landcover categories that are available for this simulation.

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[4] https://www.mrlc.gov/nlcd2011.php

Table 5-1. NLCD and MODIS land use categories for the 2022 WRF modeling

MODIS		NLCD	
Number	**Category Name**	**Number**	**Category Name**
1	Evergreen Needleleaf Forest	22	Perennial Ice/Snow
2	Evergreen Broadleaf Forest	23	Developed Open Space
3	Deciduous Needleleaf Forest	24	Developed Low Intensity
4	Deciduous Broadleaf Forest	25	Developed Medium Intensity
5	Mixed Forests	26	Developed High Intensity
6	Closed Shrublands	27	Barren Land (Rock/Sand/Clay)
7	Open Shrublands	28	Deciduous Forest
8	Woody Savannas	29	Evergreen Forest
9	Savannas	30	Mixed Forest
10	Grasslands	32	Shrub/Scrub
11	Permanent Wetlands	33	Grassland/Herbaceous
12	Croplands	37	Pasture/Hay
13	Urban And Built Up	38	Cultivated Crops
14	Cropland/Natural Vegetation Mosaic	39	Woody Wetlands
15	Permanent Snow and Ice	40	Emergent Herbaceous Wetlands
16	Barren or Sparsely Vegetated		
17	IGBP Water		

5.4 Atmospheric Data Inputs

The LADCO WRF simulation for 2022 was initialized with a blend of the 12-km (Grid #218) North American Model (NAM)[3] and the 3-km resolution High-Resolution Rapid Refresh (RAPv5/HRRRv4)[4] available from NOAA National Centers for Environmental Information (NCEI) server. These data were used to provide initial and boundary conditions (IC/BC) and input fields of the Four-Dimensional Data Assimilation (FDDA) in the WRF simulation. In addition, the Global Surface Observation Weather Data collected by the National Centers for Environmental Prediction, NCAR (NCEP)[5] was used for the surface observation grid nudging (SFDDA). FDDA refers to the nudging of the WRF simulation toward observed analyses to control model drift so that the WRF meteorological fields better represent actual historical conditions. The 3D NAM reanalysis data were downloaded from the NOAA's NCEP server and the surface HRRRv4 dataset was accessed during September 2024 from https://registry.opendata.aws/noaa-hrrr-pds.

5.5 Time Integration

Third-order Runge-Kutta integration will be used (rk_ord = 3). We set the maximum time step, defined for the outer-most domain (12 km) only, should be set by evaluating the following equation:

$$dt = \frac{6dx}{F_{map}}$$

Where *dx* is the grid cell size in km, F_{map} is the maximum map factor (which can be found in the output from the WRF program REAL.EXE), and *dt* is the resulting time-step in seconds. For the case of the 12-km domain, *dx* = 12 and F_{map} = 1.08, so *dt* should be taken to be less than 200 seconds. Longer time steps typically lead to Courant-Friedrichs-Lewy (CFL) condition errors, associated with large vertical velocity values, which tend to occur in areas of steep terrain, especially during very stable conditions in winter.

For the 2022 modeling, we used a fixed time step of 60 seconds for 12km grid domain, 20 seconds for 4km grid domain and 6.67 seconds for 1.33 km grid domain.

5.6 Diffusion Options

Horizontal Smagorinsky first-order closure (km_opt = 4) with sixth-order numerical diffusion (diff_6th_opt = 2) was used.

5.7 Lateral Boundary Conditions

Lateral boundary conditions were specified from a blend of the NAM and HRRRv4 initialization dataset on the 12 km CONUS domain with continuous updates nested from the 12-km domain to the 4-km domain and from the 4-km domain to the 1.33-km domain, using one-way nesting (feedback = 0).

5.8 Top and Bottom Boundary Conditions

The no damping option was selected for the top boundary condition and consistent with the model application for non-idealized cases, the bottom boundary condition was selected as physical, not free slip.

5.9 Sea Surface Temperature Inputs

The 6-hr interval HRRRv4 data inherently provided finer resolution skin temperature in the CONUS domain including high-resolution sea surface temperature (SST) over the Great Lakes, which is important for simulating the lake breeze dynamics in our 4-km Midwest and the 1.3-km Lake Michigan domains.

5.10 FDDA Data Assimilation

LADCO constrained the WRF model solution using a combination of analysis and surface observation nudging, i.e., FDDA. We ran the WRF model with a combination of NAM and HRRRv4 analysis and observational data for 12-km and 4-km domains only. For the grid nudging we used analysis nudging coefficients of 0.3x10-4 s -1 for horizontal winds and temperature, and a coefficient of 1.0x10-5 s -1 for water vapor mixing ratio (grid_fdda). We only applied the analysis nudging above the planetary boundary layer (Otte et al., 2008). We assimilated surface observational data in the surface grid nudging for 12-km and 4-km domains as well. The NCEP ADP Global Surface Observational Weather Data in little_r format was obtained from the Research Data Archive at the National Center for Atmospheric Research, Computational and Information Systems Laboratory (https://doi.org/10.5065/4F4P-E398, Accessed during September 2024). We applied a nudging coefficient of 0.3x10-4 s -1 for horizontal winds and temperature and a nudging coefficient of 1.0x10-5 s -1 for water vapor mixing ratio for the observation grid nudging (grid_sfdda).

5.11 WRF Physics Options

Version 4.5 of the WRF model, Advanced Research WRF (ARW) core (Skamarock, 2008) was used by LADCO for simulating 2022 meteorology. LADCO first simulated winter (January 1-15) and summer (June 15-30) test periods for eight different cases of WRF configurations and found the LADCO_WRF45_APX_NAM_HRRR6_obs case was the best performing configuration with the lowest errors and biases computed at surface monitors in the LADCO region (LADCO, 2024a). The LADCO WRF 2022 physics options included the Pleim-Xiu land surface model, the Asymmetric Convective Model version 2 planetary boundary layer scheme (Pleim 2007), Kain Fritsch cumulus parameterization (Kain 2004) utilizing the moisture-advection trigger (Ma and Tan, 2009), Morrison double moment microphysics (Morrison et al. 2005), and RRTMG longwave and shortwave radiation schemes (Gilliam and Pleim, 2010). A summary of the WRF model physics and FDDA options that LADCO used for optimizing WRF performance for the Great Lakes and central Midwest U.S. are shown in Table 5-2.

Table 5-2. Configuration options used for the LADCO 2022 WRF modeling

WRF Treatment	Option Selected	Notes
Microphysics	Thompson Scheme	mp_physics=10
Longwave Radiation	RRTMG	ra_lw_physics=4; Rapid Radiative Transfer Model (RRTM) for GCMs includes random cloud overlap and improved efficiency over RRTM.
Shortwave Radiation	RRTMG	rw_ww_physics=4; Same as above, but for shortwave radiation.
Land Surface Model (LSM)	Pleim-Xiu LSM Pleim-Xiu surface layer option	sf_surface_physics=7 sf_sfclay_physics=7
Planetary Boundary Layer (PBL) scheme	ACM2	bl_pbl_physics=7
Cumulus parameterization	Kain-Fritsch in the 12-km and 4-km domains with	cu_physics=1 and trigger_option=2; 1.33-km can explicitly simulate cumulus

	moisture-advection based trigger. None in the 1.33-km domain	convection, so parameterization is not needed.
Analysis Nudging	Aloft nudging applied to wind, temperature, and moisture in d01 and d02	Only nudging above the planetary boundary layer
Observation in grid Nudging	Surface observation nudging applied to winds, temperature, and moisture in d01 and d02	$0.3x10^{-4}$ s^{-1} (t) $0.3x10^{-4}$ s^{-1} (uv) $1.0x10^{-5}$ s^{-1} (q)
Initialization (initial and boundary conditions)	Blend of NAM218 (12-km) with surface HRRRv4 (3-km) reanalysis data in 6-hr interval	$0.3x10^{-4}$ s^{-1} (t) $0.3x10^{-4}$ s^{-1} (uv) $1.0x10^{-5}$ s^{-1} (q)

5.12 WRF Output Variables

The WRF model was configured to output additional variables to support air quality modeling with the Comprehensive Air Quality Model with Extensions (CAMx) and the Community Multiscale Air Quality Model (CMAQ). The following fields were activated in the WRF output history files: fractional land use (LANDUSEF), aerodynamic resistance (RA), stomatal resistance (RS), vegetation fraction in the Pleim-Xiu LSM (VEGF_PX), roughness length (ZNT), inverse Monin-Obukhov length (RMOL).

5.13 WRF Simulation Methodology

LADCO simulated meteorology with WRFv4.5 for the three nested domains over the U.S. on the Amazon Web Services (AWS) Elastic Compute Cloud using a distinct number of CPUs depending on pre-processing (1 node and 40 CPUs per node), actual wrf.exe simulation (4 nodes and 96 CPUs per node), and post-processing (1 node and 24 CPUs per node). The annual WRF simulation was run in quarters. Within each quarter, WRF.exe was executed in 10-day intervals. The first 10-day block of a quarter was considered as a spin-up period with each subsequent 10-day simulation initialized with a restart file from the previous 10-day simulation, effectively simulating the quarterly WRF run continuously. We used a 60 second integration time step and the results were output at 60-minute intervals. Further, the hourly WRF results were written out to 12-hour output files (2 files/day).

LADCO simulated WRF from December 22, 2021 through February 2, 2023 for the 12-km CONUS domain (d01) and the 4-km Midwest domain (d02), and from March 21, 2022 through October 31, 2022 and for all three nested domains (d01 through d03). We successfully completed the 13-month WRF simulation on all three domains in 12 wall clock days.

5.14 Evaluation Approach

LADCO conducted quantitative and qualitative analysis to assess operational performance of the 2022 WRF modeling. The quantitative model performance evaluation of WRF using surface meteorological measurement was performed using the Atmospheric Model Evaluation Tool (AMET)[5] version 1.5. AMET calculates statistical performance metrics such as bias, error, and correlation for surface winds, temperature, and mixing ratio and can produce time series of predicted and observed meteorological variables and diurnal performance statistics. For the 12-km domain modeling, which covers the entire continental U.S. and parts of Canada and Mexico, we evaluated the model performance by Multi-Jurisdictional Organization (MJO) extent. MJOs are regional organizations that provide a forum for neighboring states to collaborate on air quality planning. The focus of this WRF performance analysis was on the LADCO region. For the 4-km domain, the WRF performance was evaluated by state; and for the 1.33 domain the performance was evaluated for the entire domain. We compared modeled surface pressure, precipitation, and wind vectors against observations by season and for selected high-concentration O3 events in the Midwest. We also performed a detailed analysis of the model during lake-breeze events at the shoreline monitors of Lake Michigan.

5.15 Model Performance Evaluation

From the WRF model performance evaluation analysis, we found that the 12-km and 4-km WRF simulations adequately captured the observed meso- and synoptic-scale processes across the year in 2022. The LADCO 2022 WRF simulation represents a very close approximation of the actual meteorology that was observed in 2022. Table 5-3 shows the summer season WRF model performance mean absolute error (MAE) and mean bias (MB) for the three WRF modeling domains. While the WRF performance statistics for the 12-km and 4-km grid resolution simulations are within the acceptable performance benchmarks, the 12-km simulation has a slight cold and wet bias in the summer across much of the Eastern U.S. For the 4-km WRF simulation all the summer season metrics, except for wind direction error, fall within the simple terrain model performance benchmarks; the wind direction error falls within the complex terrain benchmark. The 1.33 km WRF simulations had very good model performance with low errors for all variables and biases near zero. Both errors and biases for temperature and specific humidity at the 12-km grid resolution are reduced by about 10% at the 4-km resolution. There was a slight degradation in model performance for the analyzed variables between the 4-km and 1.33-km resolution simulations.

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[5] http://www.cmascenter.org

Table 5-3. 2022 summer season (JJA) WRF model performance for common locations in the three LADCO WRF modeling domains

Domain	Temp2m (K)		MixingRatio2m (g/kg)		WS10m (m/s)		WD10m (degrees)	
	MAE	MB	MAE	MB	MAE	MB	MAE	MB
CONUS 12	1.2	0.0	1.1	0.3	0.9	-0.2	33.6	1.4
LADCO 4	1.1	0.2	1.0	0.5	0.9	0.0	33.4	1.7
LADCO 1.33	1.4	0.7	1.1	0.3	1.1	0.2	38.6	2.7

Analysis of WRF performance at shoreline monitors during summer season lake-breeze events showed that the model successfully reproduced the surface conditions. LADCO used a novel statistical model using data from selected surface stations on the shorelines of Lake Michigan for identifying lake-breeze days in 2022. WRF performed well predicting temperature, moisture, and winds at the shoreline monitors during lake-breeze events. The model performance is slightly better on the lake-breeze days compared to the non-lake-breeze days on shoreline of Lake Michigan. The 4-km and 1.33-km simulations had better performance simulating lake breeze conditions than the 12-km simulation. Detailed information on LADCO WRF 2022 simulation and its performance are available in the LADCO WRF 2022 modeling technical support document (LADCO, 2024b).

6 EMISSIONS

This section presents the emissions database that we will compile for the LADCO 2022 base and future year CAMx modeling simulations. Emissions data fall into three broad categories:

- Inventory data – county total estimates of emissions from explicit source categories to be processed by SMOKE to obtain the gridded hourly PGM-ready emission inputs.
- Gridded data – fluxes of emissions by grid cell or gridded data used to calculate emissions fluxes that are hourly and PGM-ready emissions inputs.
- Ancillary data – non-inventory emissions data that characterize the spatial/chemical/temporal patterns of emissions typically used with SMOKE or another emission processor to generate the hourly gridded PGM-ready emissions inputs.

Following are descriptions of these three types of data used to develop the base year and future year emissions.

6.1 Base Year 2022 Emissions

The modeling periods and domains for the LADCO 2022 modeling platform that are described above in Chapters 3 and 4 dictate the temporal and spatial coverage requirements of the 2022 emissions. We will develop an emissions modeling platform, which consists of data and software, to estimate air emissions fluxes that best represent the conditions in the LADCO region during 2022. The base 2022 modeling period is annual, starting with a model spin-up period on December 21, 2021 and ending January 31, 2023.

The following sectors will be used to represent air pollutant emissions for the LADCO 2022 modeling:

Inventory Data

- Rail
- Commercial Marine Shipping
- Airports
- Livestock
- Agricultural (fertilizer) ammonia
- Off-road mobile
- On-road mobile
- Nonpoint/Area
- Solvents
- Industrial point
- Electricity generation point
- Residential wood combustion
- Open burning
- Area and point oil and gas
- Fugitive and road dust

- Fires, including wildfires, prescribed fires, and agricultural fires
- Canada and Mexico sources

Gridded data

- Biogenic
- Sea salt

The following sections detail the sources and nature of these emissions.

6.1.1 Inventory Data

Anthropogenic emissions sources are inventoried as either point or non-point sources. Characteristics of point sources include a state/county code, plant/source/stack identifier, source classification code (SCC), and a latitude-longitude coordinate. Additional details in the point inventories are required if the sources have Continuous Emissions Monitors (CEMs) or if they are fire sources. Characteristics of non-point sources include a state/county code and SCC. Non-point sources can further be broken down into mobile and non-mobile sources, with special characteristics required for mobile sources. Descriptions of the different inventory sectors used for the LADCO 2022 modeling, including the sources of these data, are provided in this section.

All inventories for this project are from the National Emissions Collaborative (NEC) 2022[6] version 1 . The NEC publicly released the 2022v1 platform in August 2024; a 2022 version 2 platform will be released in summer 2025. A complete description of the inventory, sectors, and preparation procedures for these data are available from the U.S. EPA[7] and NEC.

Of note is that LADCO will use MOVES version 4 (MOVES4) onroad and nonroad mobile data for 2022, 2026, and 2032 in our 2022v1 emissions modeling platform. These are the best mobile source inventory data available in late 2024/early 2025.

LADCO identified unreasonably large emissions for non-point biomass (wood) boilers and engines (SCCs: 2102008000 & 2103008000) in the 2022v1 inventory for some areas in the Great Lakes region. Feedback from air program staff in the states of Ohio and Michigan believe their NSPS/permitting programs would require that any industrial, commercial, or institutional boilers that use biomass as a fuel in nonattainment counties would require an operating permit. These sources would be included in their point source inventory submission to the NEI and should not be included as nonpoint sources in the 2022v1 platform.

LADCO worked with staff from Ohio and Michigan on a solution that redistributes the emissions from nonattainment counties to attainment counties in their states, ensuring no emissions are removed from the statewide emissions inventory. LADCO updated the 2022v1 nonpoint inventory by redistributing the emissions for biomass-fueled boilers from nonattainment counties in Michigan

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[6] http://views.cira.colostate.edu/wiki/wiki/9169

[7] https://www.epa.gov/air-emissions-modeling/2022v1-emissions-modeling-platform

and Ohio to attainment counties in equal proportions to existing estimates. The nonattainment counties impacted by this change include:

- Michigan: Allegan, Berrien, Livingston, Macomb, Monroe, Muskegon, Oakland, St. Clair, Washtenaw, and Wayne
- Ohio: Butler, Clermont, Cuyahoga, Delaware, Fairfield, Franklin, Geauga, Hamilton, Lake, Licking, Lorain, Medina, Portage, Summit, and Warren. The table below shows the NOX and PM2.5 impacts by state.

Table 6-1 shows the impact of redistributing the biomass boiler emissions from nonattainment to attainment counties in Michigan and Ohio.

Table 6-1. Biomass Boiler Emissions Changes by State, SCC, Pollutant, and Attainment status

State	SCC	Pollutant	County Attainment Status	2022v1 Annual Emissions	2022v1 Annual Updated Emissions
MI	2102008000	NOX	Attainment	898	1,748
MI	2102008000	NOX	Non-attainment	850	0
MI	2102008000	PM25-PRI	Attainment	1,825	3,551
MI	2102008000	PM25-PRI	Non-attainment	1,726	0
MI	2103008000	NOX	Attainment	224	537
MI	2103008000	NOX	Non-attainment	313	0
MI	2103008000	PM25-PRI	Attainment	454	1,090
MI	2103008000	PM25-PRI	Non-attainment	636	0
OH	2102008000	NOX	Attainment	640	1,200
OH	2102008000	NOX	Non-attainment	561	0
OH	2102008000	PM25-PRI	Attainment	1,300	2,439
OH	2102008000	PM25-PRI	Non-attainment	1,139	0
OH	2103008000	NOX	Attainment	139	379
OH	2103008000	NOX	Non-attainment	240	0
OH	2103008000	PM25-PRI	Attainment	282	770
OH	2103008000	PM25-PRI	Non-attainment	489	0
	Total Emissions			**11,715**	**11,715**

LADCO will break the 2022 inventory sectors into processing sectors to facilitate reporting, quality assurance, and special processing of the data. Table 6-2 lists the major anthropogenic emission inventory sectors used for the LADCO 2022 modeling. This table includes fires in addition to the anthropogenic inventories. The data source of all sectors shown in Table 6-2 is the NEC 2022v1, except where noted otherwise.

Table 6-2. LADCO 2022 inventory sectors

Sector	Inventory Type	Inventory Period	Description
Rail	Nonpoint	Monthly	The rail sector includes county-level emissions for locomotives (nonpoint) and train yards (point)
Airports	Point	Daily	Point source inventory of 20,000 airports using Federal Aviation Administration's (FAA's) Aviation Environmental Design Tool (AEDT) with daily landing and takeoff data for each airport.
Class 1 & 2 Commercial Marine Vessels (CMV)	Nonpoint	Monthly	The CMV sector includes emissions as point sources for class 1 and 2 in- and near-shore commercial marine; the points are located at the center of a U.S. EPA data grid derived from CMV automatic identification system data for 2022
Class 3 CMV	Point	Annual	Elevated point CMV sources for class 3 vessels in offshore commercial shipping lanes; the points are located at the center of a U.S. EPA data grid derived from CMV automatic identification system data for 2022
Off-road mobile	MOVES4	Monthly	MOVES4 county-level inventories for recreational vehicles, logging equipment, agricultural equipment, construction equipment, industrial equipment, lawn and garden equipment, leaf and snow blowers, and recreational marine.
On-road mobile	MOVES4	Annual and Daily	EPA ran MOVES4 for 2022 in emissions factor mode. The MOVES lookup tables include emissions for the following processes, each of which represents an explicit processing sector in SMOKE: Rate-per-distance (RPD) for running exhaust, Rate-per-hour (RPH) for truck hoteling, Rate-per-hour for off-network (RPHO) idling, Rate-per-profile (RPP) for diurnal evaporative, Rate-per-start (RPS), Rate-per-vehicle (RPV) for running evaporative. These data include the reference county and reference fuel month assignments that U.S. EPA used for the MOVES simulation. The emissions rate method was also used with state specific methods for California. The California MOVES estimates were normalized to emissions values provided by CARB. This also includes updates for temporalization for speed and VMT based on telematics data.
Non-point/ Area	Nonpoint	Annual	County-level emissions for sources that individually are too small in magnitude or too numerous to inventory as individual point sources.

Sector	Inventory Type	Inventory Period	Description
Livestock	Nonpoint	Annual	Used the Emissions Model (FEM) developed by Carnegie Mellon University (CMU) and updated USDA animal population representing the year 2020.
Residential Wood Combustion	Nonpoint	Annual	Based on U.S. EPA residential wood emissions tool.
Open Burning	Nonpoint	Annual	This sector includes land clearing, residential household waste, and yard waste.
Livestock	Nonpoint	Annual	Based on U.S. EPA's Agricultural Sources Emissions inventory derived from Carnegie Mellon University emissions rates and 2020 populations.
Fertilizer	Nonpoint	Annual	Created with Fertilizer Emissions Scenario Tool for CMAQ (FEST-C)
Solvents	Nonpoint	Annual	Diverse collection of solvent use for residential, commercial, institutional, and industrial sources
Nonpoint Oil & Gas	Nonpoint	Annual	The non-point O&G sector includes non-permitted sources used for up-stream exploration, development, and production
Point Oil & Gas	Point	Annual	The point O&G sector includes permitted sources used for up-stream exploration, development, and production
Electricity Generation Unit (EGU) Point	Point	Hourly	Combination of NEC2022v1 and 2022 Clean Air Markets Division (CAMD) hourly Continuous Emissions Monitor (CEM) data for the base year and ERTAC projections for future years.
non-EGU (Industrial) Point	Point	Annual	Elevated and low-level combustion and industrial sources, rail yards, and offshore drilling platforms.
Area Source Dust	Nonpoint	Annual	Road construction, paved roads, and unpaved roads.
Fires	Point	Hourly	The SMOKE processing sectors for fires include: hourly agricultural, prescribed, and wildfire sources with pre-computed plume parameters and speciated PM.
Canada Sources	Nonpoint and Point	Annual	The Canadian 2015 National Pollutant Release Inventory (NPRI) includes SMOKE processing sectors fugitive dust, oil and gas, onroad, nonroad, agriculture, non-point, and industrial Point
Mexico Sources	Nonpoint and Point	Annual	The Mexican NEI 2008 Inventory (INEM) projected to 2014 includes SMOKE processing sectors for industrial point, agriculture, dust, non-point, and mobile

6.1.2 Gridded Data

Several gridded datasets are used to either directly estimate air emissions or they are used as ancillary data for processing/adjusting the emissions data. The following datasets are key gridded data used for the LADCO 2022 modeling.

Biogenic Emissions Model Inputs

The major components of biogenic emissions models include:

- Leaf Area Index (LAI)
- Plant Functional Type (PFT)
- Plant specific species composition data and averaging
- Emissions factors, including the effects of temperature and photosynthetically active radiation (PAR)

Sea Salt

Ramboll developed an emissions processor that integrates published sea spray flux algorithms to estimate sea salt PM emissions for input to CAMx. The gridded data for input to the sea salt emissions model used for the LADCO 2022 modeling is a land-water mask file that identifies each modeling domain grid cell as open ocean, surf zone, or land.

LADCO will use the CAMx sea salt emissions processor with 2022 WRF data to generate sea salt emissions for the 12 km modeling domain. The LADCO 4 km domain does not have any sea salt emissions sources

Fugitive Dust Transport Factors

We will apply transport factors to the primary dust emissions estimates to adjust the emissions for vegetative scavenging, soil moisture, and snow cover. The dust models and emissions factors are based on soil characteristics and do not account for the presence of vegetation or precipitation, both of which have a mitigating effect on dust emissions. LADCO will apply an ad-hoc approach of adjusting dust emissions estimates that uses gridded land cover data and meteorology to simulate the impacts of vegetation and precipitation on dust.

We will use the U.S. EPA fugitive dust correction factors that are derived from the 2016 WRF model runs using the gen_afdust_tfrac tool and the Biogenic Emission Landuse Database version 3 (BELD3; Vukovich and Pierce, 2002) Following the approach of Pouliot et al. (2010), we will adjust the fugitive and road dust emissions as a post-processing step after the emissions data are output from SMOKE. We will use dust transport factors gridded to each of the LADCO modeling domains to reduce the dust emissions. The values of the transport factors associated with each BELD3 land cover category are available in Pouliot et al.

6.1.3 Ancillary Emissions Data

Ancillary emissions data includes all the factors and support files required to convert inventory and gridded data to the input formats and terms expected by a PGM, including:

Spatial data. All anthropogenic non-point inventory data, except on-road mobile sources, are estimated at the county level. Gridded hourly on-road mobile source emissions will be estimated using the SMOKE-MOVES processor with MOVES emissions factor lookup tables and hourly gridded meteorology from the LADCO 2022 WRF meteorological modeling. The county-level emission inventories are mapped to the model grid cells using data files containing spatial surrogates. Spatial surrogate files are generated with software that uses Geographic Information System (GIS) Shapefiles to calculate the fraction of the county total activity within a model grid cell based on geospatial attributes. For example, a Shapefile of the housing distribution in Cook County, IL will assign the appropriate percentage of Cook County housing to each grid cell in the county. This information allows us to allocate county-level emission inventory sources that are associated with housing (e.g.) to the modeling grids.

Spatial surrogates require cross-referencing data that assign a spatial surrogate to specific categories of inventory sources. Spatial cross-reference files assign surrogates to inventory sources using country/state/county codes (FIPS) and source classification codes (SCCs).

Temporal data. Air quality modeling systems, such as CMAQ and CAMx, require hourly emissions input data. There are a few exceptions (e.g. Continuous Emissions Monitoring data, biogenic emissions, windblown dust and some fire inventories), but most inventory data include annual or daily emission estimates. To compute hourly emissions from the annual or daily inventory estimates, the SMOKE model uses three types of temporal profiles:

1. Monthly profiles: Convert annual inventory to monthly emissions accounting for seasonal and other effects.
2. Daily profiles: Convert monthly emissions to daily emissions accounting for day-of-week and other effects.
3. Hourly profiles: Convert daily emissions to hourly emissions accounting for the diurnal variation in emissions (e.g., work schedules and commute times).

Temporal profiles are assigned to inventory sources using cross-referencing data that match the profiles and inventory sources using country/state/county (FIPS) and source classification codes (SCCs).

Chemical speciation data. Emissions inventories have limited chemical composition information. For this project, LADCO will use chemical speciation profiles to partition emission inventories that contain six criteria pollutants: carbon monoxide (CO), nitrogen oxides (NO_X), volatile organic compounds (VOC), ammonia (NH_3), sulfur dioxide (SO_2), particulate matter with a mean diameter < 10 micrometers (PM_{10}), and particulate matter with a mean aerodynamic diameter less than 2.5 micrometers ($PM_{2.5}$). Chemical speciation profiles will be used to describe the chemical composition of the effluent from emissions sources. The chemistry mechanism selected for the AQM simulation dictates the exact specification of the source-specific chemical species. For example, a speciation profile exists that converts the inventory pollutant NO_X to the PGM input species NO, NO_2, and HONO. Speciation profiles are required to partition four (NO_X, VOC, SO_2, and $PM_{2.5}$) of the six inventory pollutants into PGM species. LADCO will partition VOC to the species required by the CB7r1ae7 chemical mechanism using source specific speciation profiles developed from the SPECIATE 5.3 database.

Chemical speciation profiles are assigned to inventory sources using cross-referencing data that match the profiles and inventory sources using country/state/county (FIPS) and source classification codes (SCCs).

LADCO will take the base set of ancillary data directly from the NEC 2022v1 platform. LADCO will make targeted improvements to the ancillary data files for the LADCO states. We will focus our improvements on the assignments of spatial/chemical/temporal profiles to the largest inventory sources and on developing profiles that best represent the emissions patterns in the LADCO region.

By targeting the largest emissions sources (e.g., top 90% of annual NOx and VOC emitters in each LADCO state), we will maximize the improvement effort by limiting the number of sources to those with the largest impact on air quality.

6.2 Future Year Emissions

We will prepare a future year modeling platform with inventories projected to 2026 and 2032 using information on emissions growth and controls from the year 2022 forward. The inventory data for the LADCO future year modeling platforms will come primarily from the NEC 2022v1 platform and from the U.S. EPA. Electricity Generating Unit (EGU) forecasts will be generated by the ERTAC EGU working group.

Developed by the NEC for use in expected upcoming SIP applications, the 2022v1-based projections to 2026 and 2032 were the best estimate of future year emissions available at the time this report was written.

Below is a summary of the 2022 modeling platform projections.

- CEM Point: Unit-specific hour-specific estimates from ERTAC EGU Model version 22.1.
- Non-CEM Point: Projection factors and percent reduction to reflect comments and emission reductions due to national and local rules, control programs, plant closures, consent decrees and settlements. Terminal area forecast (TAF) data aggregated to the national level to account for projected changes in landing/takeoff activity for aircraft.
- Point and nonpoint oil and gas sectors: For upstream oil and gas sources, regional projection factors by product type using Annual Energy Outlook (AEO) 2023 projections to year 2026, 2032, and 2038. Co-benefits of stationary engines CAP-cobenefit reductions (RICE NESHAP) and New Source Performance Standards (NSPS) VOC controls reflected for select sources.
- Nonpoint/Area: Agricultural sector projection factors for livestock estimates based on expected changes in animal population from 2023 AEO. Fertilizer application NH_3 emissions projections include upstream impacts EISA. Fugitive dust projection factors for dust categories related to livestock estimates based on expected changes in animal population and upstream impacts from EISA. Other projection factors that implement Cross State Air Pollution Rule comments and reflect emission reductions due to control programs. Residential wood combustion projections based on projection factors that reflect assumed growth of wood burning appliances based on sales data, equipment replacement rates and change outs. These changes include growth in lower-emitting

stoves and a reduction in higher emitting stoves. PFC projection factors reflecting impact of the final Mobile Source Air Toxics (MSAT 2) rule. Upstream impacts from EISA, including post-2007 cellulosic ethanol.

- Off-road Mobile: Other than for California, this sector data comes from a U.S. EPA application of MOVES4 that uses future-year equipment population estimates and control program inputs supplied by state as part of the 2020NEIv1 development or national-level inputs. Controls from the final locomotive-marine and small spark ignition OTAQ rules are included. The California Air Resources Board (CARB) provided California-specific data.
- Locomotive/marine: For all states except California, projection factors for Class 1 and Class 2 commercial marine and locomotives reflect final locomotive-marine controls and RFS2 adjustments. Growth rates for rail will use AEO projection factors and updated fleet mix based on ERTAC rail group methodologies.
- Offshore shipping: Base-year 2022 emissions grown and controlled to 2026, 2032, and 2038, incorporating controls based on Emissions Control Area (ECA) and International Marine Organization (IMO) global NO_X and SO_2 controls.
- On-road Mobile, not including refueling: MOVES4 (extended idle mode) and MOVESTier3NPRM-based emissions factors for years 2026, 2032, and 2038 use the same representative counties, state-supplied data, meteorology, and procedures that were used to produce 2022 emission factors. CARB provided California-specific data. This sector includes all non-refueling on-road mobile emissions (exhaust, extended idle, evaporative, evaporative permeation, brake wear and tire wear modes).
- On-road Refueling: Uses the same projection and processing approach as the on-road sector, except for California, where U.S. EPA projected using MOVES4 and did not include CARB data.
- Canada Sources: Held constant at 2020 levels
- Mexico Sources: Projections from 2018 to 2026, 2032, and 2038

We will not make any changes to the ancillary emissions data (spatial/temporal/chemical) for the future year emissions. These data will be held constant at the 2022 values when preparing the future year emissions for CAMx.

6.3 Emissions Processing

We will use SMOKE version 5.1 (July 2024) for processing the 2022-based emissions. SMOKE will be used to process all the emissions sectors other than biogenics, sea salt, and lightning. Listed below are the primary steps in the SMOKE processing sequence, with the name of the SMOKE program. We provide the significant SMOKE configuration options along with each step.

6.3.1 SMOKE Processing

The procedures for processing the emissions for generating CAMx emission inputs using SMOKE are described below. LADCO will use modified versions of the U.S. EPA Emissions Modeling Framework (EMF)-based SMOKE scripts to process the 2022v1 emissions.

Import Inventories to SMOKE

- SMOKE Program: Smkinven
- Primary Function: read raw inventory files
- Settings:
  - Calculate coarse mode primary particulate matter (PMC) emissions, where SMKINVEN_FORMULA: PMC = PM10-PM2.5;
  - For the hourly CEM inventories, set to read hourly data, where HOUR_SPECIFIC_YN = Y;
  - Do NOT normalize weekly emissions by weekdays only, where WKDAY_NORMALIZE = N;
  - Do NOT process hazardous air pollutant emissions, where SMK_PROCESS_HAPS = N;

Distribute Inventories to Model Grid Cells

- SMOKE Program: Grdmat
- Primary Function: read and match spatial surrogates to inventory sources and assign the emissions to PGM grid cells
- Settings:
  - For all sources other than agriculture, use population as the fallback surrogate, where SMK_DEFAULT_SRGID = 100;
  - For livestock and fertilizer, use rural land area as the fallback surrogate, where SMK_DEFAULT_SRGID = 400;
  - Process all sources on a normal sphere with radius 6,370,000 m, where IOAPI_ISPH = 20;

Chemical Speciation

- SMOKE Program: Spcmat
- Primary Function read and match VOC and PM chemical profiles to inventory sources and calculate emissions in terms of PGM species
- Settings
  - Convert inventory VOC to total organic gases (TOG) for consistency with the NEI SPECIATE speciation profiles, where POLLUTANT_CONVERSION = Y;

Estimate Hourly Emissions

- SMOKE Program: Temporal
- Primary Function: read and match monthly/week/hourly temporal profiles to inventory sources and estimate hourly emissions
- Settings:
  - Renormalize the temporal profiles, where RENORM_TPROF = Y;

  - Do NOT force all temporal profiles to be flat, where UNIFORM_TPROF_YN = N;
  - Output emissions on the GMT time zone, where OUTZONE = 0;
  - Select elevated sources (Elevpoint) – read criteria for specifying elevated point sources;
  - Use a configuration file to select elevated sources, where SMK_ELEV_METHOD = 1;
  - All point sources for the LADCO modeling are considered elevated if the effective stack height is greater than 20m;

Create CAMx-ready Emissions

- SMOKE Program: Smkmerge
- Primary Function: combine all the intermediate steps above to create a low-level emissions file for each inventory sector and an elevated file for the elevated point sectors
- Settings:
  - Combine gridding, temporal, and speciation intermediates to create PGM-ready emissions, where MRG_GRDOUT_YN = MRG_TEMPORAL_YN = MRG_SPCMAT_YN = Y;
  - Output an elevated file that includes the emissions for elevated sources, where SMK_ASCIIELEV_YN = Y;
  - Output emissions in CAMx units, where MRG_GRDOUT_UNIT = moles/hr;

Estimate On-Road Mobile Emissions from MOVES

- SMOKE Program: MOVESMrg
- Primary Function: input mobile activity data and MOVES emission factor look up tables to generated gridded, speciated, hourly emissions
- Settings:
  - Process MOVES emissions, where SMK_EF_MODEL = MOVES;
  - Use 2-m temperatures for processing the on-road mobile emissions, where TVARNAME = TEMP2;
  - Extend a 10-degree temperature buffer on either side of the emissions factor look up tables, where TEMP_BUFFER_BIN = 10;

Create CAMx-ready binary files

- SMOKE Program: Smk2emis
- Primary Function: convert netCDF SMOKE outputs to UAM-formatted data for CAMx

LADCO will define a series of emissions processing categories for the 2022 modeling project to facilitate the modeling and quality assurance of the inventory data. LADCO has defined these categories to support special emissions modeling approaches or to provide flexibility for tagging emissions categories in source apportionment air quality modeling.

Efficiencies in the emissions modeling process are gained through consideration of the temporal variability in the emissions sources. If a processing category includes only sources that use a flat temporal profile throughout the year, meaning that the emissions are the same on every hour of every day of the year, it is possible to process a single day for that category and recycle the emissions on each day of the air quality modeling simulation. Both processing time and disk space are conserved by not producing 365 files that all contain the exact same information. Other types of temporal processing configurations that may be used for this project include:

- Single day per year (aveday_yr)
- Single day per month (aveday_mon)
- Typical Monday, Weekday, Saturday, Sunday per year (mwdss_yr)
- Typical Monday, Weekday, Saturday, Sunday per month (mwdss_mon)
- Emissions estimated for each model simulation day (daily)
- Emissions estimated for each model simulation day with temporal profiles generated with average daily meteorology (daily met)
- Emissions estimated for each model simulation day with temporal profiles generated with hourly meteorology (hourly met)

6.3.1 Sea salt Emissions Processing

Sea salt emissions will be calculated internally (in-line) in CAMx during the simulation.

6.4 Quality Assurance and Quality Control

LADCO will process the emissions by major source category in several different “streams” of emissions modeling to assist in the quality assurance (QA) and quality control (QC) of the emissions modeling. Each stream of emissions modeling generates a pre-merged CAMx-ready emissions model input. New versions of CAMX can read in all the separate emissions input files so that a merged file of low-level sources is not needed. Table 6-2 lists the separate streams of emissions modeling by source category to be used by LADCO.

7 PHOTOCHEMICAL MODELING

LADCO will conduct photochemical modeling using the CAMx photochemical grid model (PGM).

The PGM model simulations will initially be conducted for two emission scenarios:

- 2022 base case modeling that is used in the model performance evaluation and to define baseline air quality conditions.
- 2026 and 2032 future year modeling for estimating the change to air quality under future year emissions conditions

The LADCO CAMx modeling will provide the framework for 2022-based planning modeling needed to support O_3 and $PM_{2.5}$ State Implementation Plans for the LADCO states. This chapter describes the model configurations for the CAMx 2022 base and 2026 and 2032 future year simulations. Except for the emissions input files, the base and future year simulation CAMx configurations are the same. Chapter 8 describes the procedures for evaluating performance of the model for the 2022 simulation.

We will include an addendum to this protocol to address any additional sensitivity modeling required to address model performance issues or to develop emissions control strategies as directed by the Technical Oversight Committee (TOC) and/or the Air Directors.

7.1 CAMx Science and Input Configurations

Tables 7-1 summarizes the CAMx science configurations and options to be used for the 2022 base case simulations. In general, LADCO will base the CAMx air quality modeling platform for this study on the configuration that we used for our recent 2015 O3 NAAQS Transport Modeling (LADCO, 2018) and the regional haze modeling conducted for the reasonable progress for the Regional Haze Rule second planning period (LADCO, 2021). The LADCO modeling was based on work done by the U.S. EPA to support both their October 2017 memo on Interstate Transport SIPs for the 2008 Ozone NAAQS (USEPA, 2015) and their December 2016 technical support document on a preliminary assessment of Interstate Transport for the 2015 Ozone NAAQS (U.S. EPA, 2016). However, LADCO will run CAMx v7.31 (Ramboll, 2024) as the photochemical grid model (PGM) for this application.

CAMx is a three-dimensional, Eulerian air quality model that simulates the chemical transformation and physical transport processes of air pollutants in the troposphere. It includes capabilities to estimate the concentrations of primary and secondary gas and particle phase air pollutants, and dry and wet deposition, from urban to continental spatial scales. As CAMx associates source-level air pollution emissions estimates with air pollution concentrations, it can be used to design and assess emissions reduction strategies pursuant to NAAQS attainment goals.

We will use the PPM advection solver for horizontal transport (Colella and Woodward, 1984) along with the spatially varying (Smagorinsky) horizontal diffusion approach. CAMx will use K-theory for vertical diffusion using the CMAQ-like vertical diffusivities from WRFCAMx. The CB7r1 gas-phase chemical mechanism is selected for CAMx because it includes the latest knowledge on ozone chemistry of biogenic VOCs and an updated iodine mechanism for ozone destruction. Moreover, the secondary organic aerosol chemistry/partitioning module (SOAP3) was substantially revised the formation of organic condensable gases and aerosols from VOC/IVOC/SVOC precursors.

Additional CAMx inputs will be as follows:

Meteorological Inputs: WRF-derived meteorological fields processed with WRFCAMx version 5.2 to generate CAMx meteorological inputs, as described in Chapter 5.

Initial/Boundary Conditions: 2022 chemical boundary conditions for the 12-km continental U.S. modeling domain derived from U.S. EPA northern hemisphere CMAQ simulations of 2022[8]. The U.S. EPA 2022 ICBCs are hourly, vertically resolved up to 50 mb, and used the Carbon Bond mechanism(cb6r5ae7).

Photolysis Rates: total ozone column and clear-sky photolysis rate inputs prepared by LADCO for CAMx. Day-specific O_3 column data of -the satellite-based Ozone Monitoring Instrument (OMI) was obtained from NASA (https://acd-ext.gsfc.nasa.gov/anonftp/toms/omi/data/Level3e/ozone). Daily data will include gaps of missing data due to the limited coverage of the OMI instrument. These gaps are automatically filled by the O3MAP program using interpolation (o3map version 3.1).

The TUV photolysis rate processor version 4.8 will be used for preparing a clear-sky photolysis rate input file for the CAMx version 7.31. Starting with CAMx v6.0, the TUV radiative transfer and photolysis model, developed and distributed by the National Center of Atmospheric Research (NCAR, 2011), is used as a CAMx preprocessor to provide the air quality model with a multi-dimensional lookup table of clear-sky photolysis rates. CAMx internally adjusts clear-sky rates for the presence of clouds and aerosols using a fast in-line version of TUV.

Land-use, topographic elevation, and leaf area index data: these data will be derived from the LADCO WRF 2022 outputs.

Spin-Up Initialization: A minimum of ten days of model spin up (e.g., December 21-31, 2021) will be used on the 12-km CONUS domain and 4-km nested Midwest domain.

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[8] s3://epa-2022-modeling-platform/bcon/HEMI_CMAQ_12US2_CAMxBC

Table 7-1. LADCO 2022-based CAMx (Version 7.31) model configuration.

Science Options	Configuration	Details
Model Codes	CAMx v7.31	
Horizontal Grid Mesh	12-km and 4-km	
12 km grid	396 col x 246 rows	
4 km grid	420 col x 390 rows	
Vertical Grid Mesh	Full 36 layers as in WRF outputs	
Grid Interaction	None	
Initial Conditions	10-day spin-up on 12 km grid	Clean initial conditions at the start of the model spin-up period
Boundary Conditions	12-km from hemispheric CMAQ	
Emissions		
Baseline Emissions Processing	SMOKE, MOVES4, and BEIS4	
Sub-grid-scale Plumes	None	
Chemistry	True	
Wet Deposition	True	
Gas Phase Chemistry	CB7r1	Carbon Bond 7 revision 1
Aerosol Chemistry	CF3	Static Course and Fine modes with ISORROPIA inorganic gas-aerosol partitioning, SOAP3 organic gas-aerosol partitioning and oxidation
Meteorological Processor	WRFCAMx_v5.2	Compatible with CAMx V7.30
Horizontal Diffusion	Spatially varying	K-theory with Kh grid size dependence
Vertical Diffusion	CMAQ-like in WRF2CAMx	KVPatch was not used
Diffusivity Lower Limit	Kz_min = 0.1 to 1.0 m^2/s or 2.0 m^2/s	Land use dependent
Deposition Schemes		

Dry Deposition	Zhang dry deposition scheme (CAMx)	Zhang et al. 2003
Wet Deposition	True	CAMx-specific formulation for rain/snow/graupel/virga
Bidi_NH3_Drydep	False	
Numeric Solvers		
Gas Phase Chemistry Solver	Euler Backward Iterative (EBI) -- Fast Solver	
Vertical Advection Scheme	Implicit scheme w/ vertical velocity update (CAMx)	
Horizontal Advection Scheme	Piecewise Parabolic Method (PPM) scheme	PPM Scheme (Colella and Woodward, 1984)
Integration Time Step	Wind speed dependent	~0.1-1 min (4 km), 1-5 min (12--km)

8 MODEL PERFORMANCE EVALUATION

This chapter describes the general model performance evaluation procedures that are designed to estimate the reliability of the CAMx models for simulating air quality, visibility and deposition in the LADCO region for the 2022 modeling period. LADCO will first evaluate model performance for O_3 and $PM_{2.5}$. If the initial model performance seems reasonable, we will conduct a more detailed model performance evaluation that also includes precursors, product, and indicator species of O_3 and $PM_{2.5}$.

8.1 Overview of Model Performance Evaluation

Using the inputs and model configurations described in this Modeling Protocol, an initial CAMx base case simulation will be conducted for the 12 and 4 km domains and selected 1-2 week periods during the winter and summer of 2022. The initial 2022 base case O_3, total $PM_{2.5}$ mass and speciated $PM_{2.5}$ concentrations will be evaluated against concurrent measured ambient concentrations using graphical displays of model performance and statistical model performance measures that would be compared against established model performance goals and criteria. The CAMx performance evaluation will follow the procedures recommended in U.S. EPA's photochemical modeling guidance documents (U.S. EPA, 2018b).

After an initial overview of the model performance evaluation focusing on O_3 and $PM_{2.5}$ is performed, a more detailed model performance evaluation on the annual CAMx simulation will be conducted that also includes O_3/$PM_{2.5}$ precursor species, including NO, NO_2, NO_X, total VOCs, speciated VOCs (where available), SO_2, and NH_3.

8.2 Available Aerometric Data for the model Evaluation

LADCO will utilize routine air quality measurement data networks that operated in 2022 to assess CAMx model performance:

EPA AQS Surface Air Quality Data: Data files containing hourly-averaged concentration measurements at a wide variety of state and U.S. EPA monitoring networks are available in the Air Quality System (AQS) database throughout the U.S. The AQS consists of many sites that tend to be mainly located in and near major cities. These data sets will be reformatted for use in the model evaluation software tools and used in the regional evaluation of the modeling system. There are several types of networks within AQS that measure different species. The standard hourly AQS AIRS monitoring stations typically measure hourly O_3, NO_2, NO_X and CO concentration and there are thousands of sites across the U.S.

The Federal Reference Method (FRM) network for PM measures 24-hour total $PM_{2.5}$ mass concentrations using a 1:3-day sampling frequency, with some sites operating on an everyday frequency. The Chemical Speciation Network (CSN) measures speciated $PM_{2.5}$ concentrations including SO_4, NO_3, NH_4, EC, OC and elements at 24-hour averaging period using a 1:3 or 1:6-day sampling frequency. Figure 8-1 and Figure 8-2 show the locations of the FRM and CSN monitoring networks, respectively, the AIRS hourly network is not shown because the large number of sites makes the map unreadable.

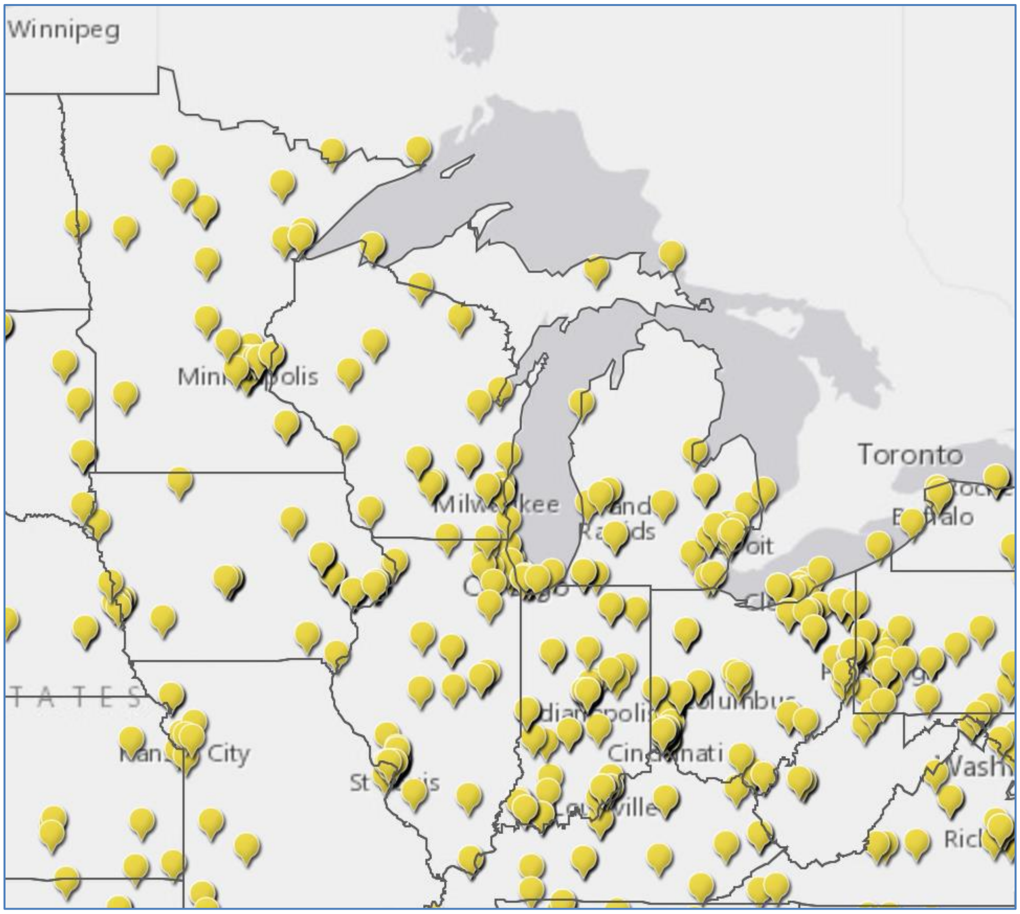

Figure 8-1. Locations of FRM PM$_{2.5}$ mass monitoring sites in the LADCO region

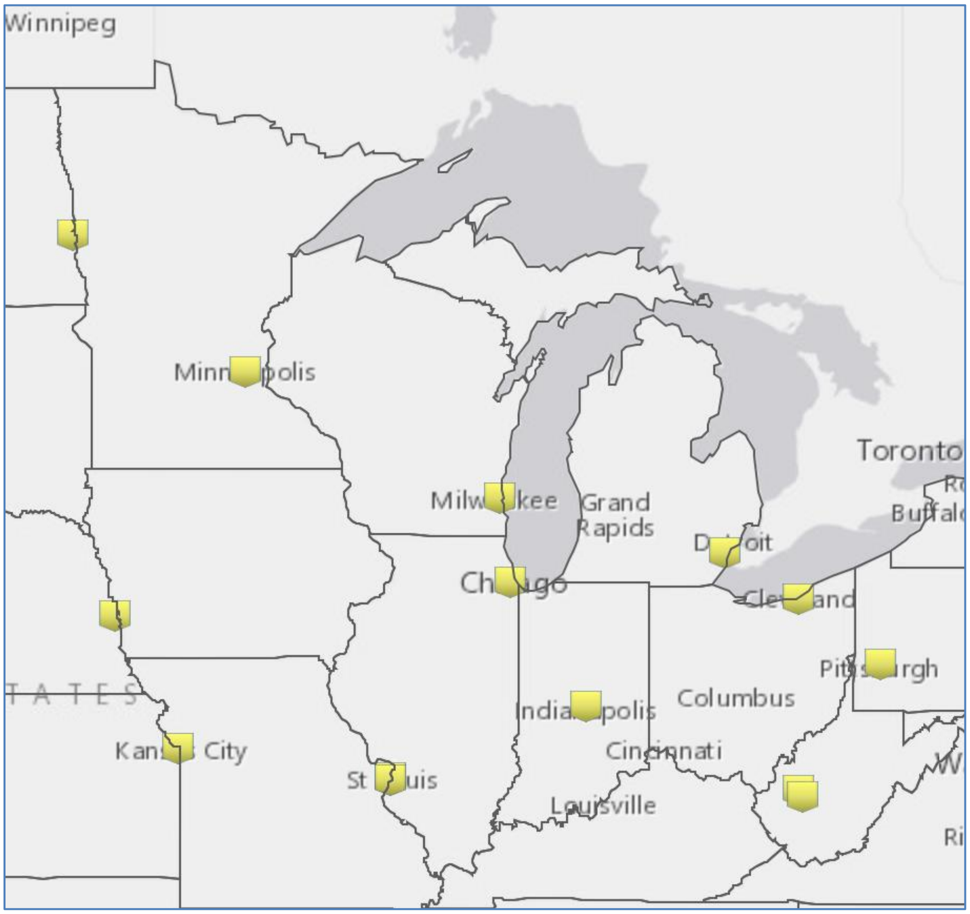

Figure 8-2. Locations of CSN speciated PM$_{2.5}$ monitoring sites in the LADCO region

IMPROVE Monitoring Network: The Interagency Monitoring of Protected Visual Environments (IMPROVE) network collects 24-hour average PM$_{2.5}$ and PM$_{10}$ mass and speciated PM$_{2.5}$ concentrations (with the exception of ammonium) using a 1:3 day sampling frequency. IMPROVE monitoring sites are mainly located at more rural Class I area sites that correspond to specific National Parks, Wilderness Areas and Fish and Wildlife Refuges across the U.S. with many sites located in the western U.S. Additionally, there are also some IMPROVE protocol sites in urban areas and rural areas not designated as Class I areas. Figure 8-3 shows the locations of the approximately 150 IMPROVE and IMPROVE protocol sites across the U.S.

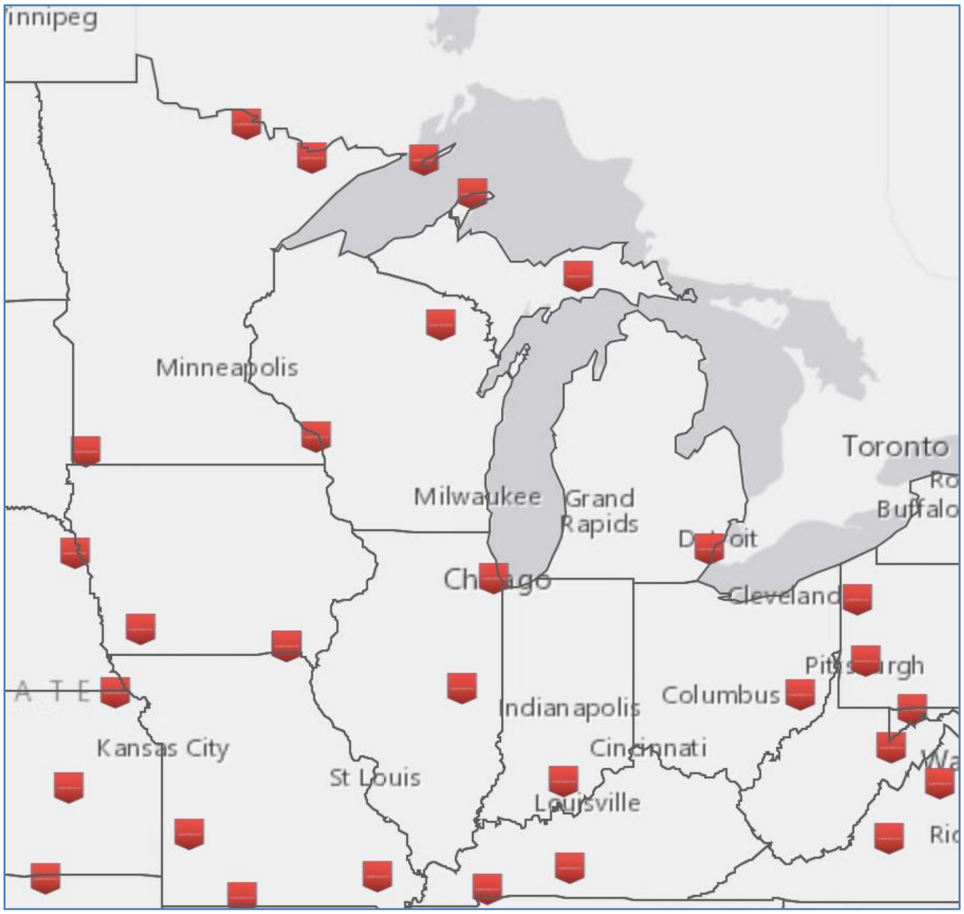

Figure 8-3. Locations of IMPROVE speciated $PM_{2.5}$ monitoring sites in the LADCO region

CASTNet Monitoring Network: The Clean Air Status and Trends Network (CASTNet) operates approximately 80 monitoring sites in mainly rural areas across the U.S. CASTNet sites typically collect hourly O_3, temperature, wind speed and direction, sigma theta, solar radiation, relative humidity, precipitation and surface wetness. CASTNet also collects weekly (Tuesday to Tuesday) samples of speciated $PM_{2.5}$ sulfate, nitrate, ammonium and other relevant ions and weekly gaseous SO_2 and nitric acid (HNO_3). Figure 8-4 displays the locations of the approximately 80 CASTNet sites across the U.S.

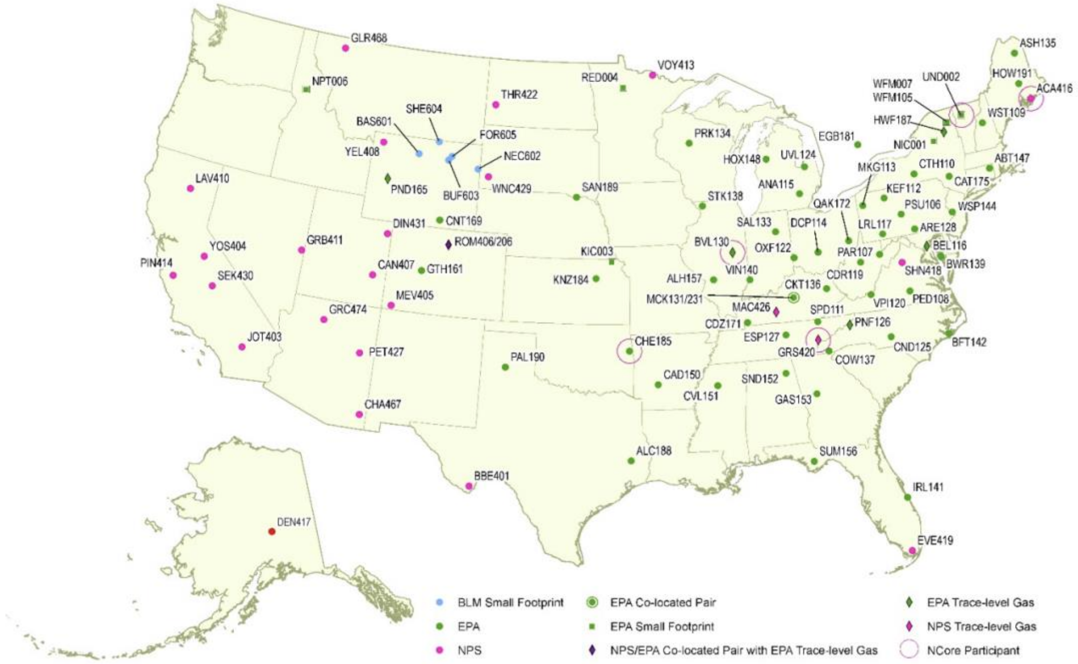

Figure 8-4. Locations of CASTNet monitoring sites; source: https://www.epa.gov/castnet

8.3 Model Performance Statistics, Goals and Criteria

U.S. EPA (2018) recommended a 60 ppb observed O_3 cut-off threshold when calculating O_3 model performance statistics. Emery et al., (2017) conducted a meta-analysis of 38 peer-reviewed articles from 2005 through 2015 on photochemical grid modeling applications to update the MPE benchmarks for O_3 and particulate matter modeling. Table 8-1 lists their recommended MPE goals and criteria, and cutoff concentrations. In addition, Emery et al., recommended that MPE statistics for O_3 should be calculated for time periods of roughly 1 week (episodic) and not to exceed 1 month.

Table 8-1. Ozone model performance benchmarks by Emery, et al. (2017)

Metric	Goal	Criteria	Cutoff
Normalized Mean Bias (NMB)	≤± 5%	≤± 15%	40 ppb for 1-hour O_3, no cutoff for MDA8 O_3
Normalized Mean Error (NME)	< 15%	< 25%	40 ppb for 1-hour O_3, no cutoff for MDA8 O_3
Correlation Coefficient (r)	> 0.75	> 0.5	No cutoff

U.S. EPA's modeling guidance (U.S. EPA, 2018) notes that PM models might not be able to achieve the same level of model performance as O_3 models. Indeed, $PM_{2.5}$ species definitions are defined by the measurement technology used to measure them and different measurement technologies can produce very different $PM_{2.5}$ concentrations. Given this complexity, researchers have developed PM model performance goals and criteria that are less stringent than the O_3 goals as shown in Table 8-2 (Boylan, 2006; Morris et al., 2005). For PM species the Fractional Bias (FB) and Fractional Error (FE) are utilized with no observed concentration threshold screening. The FB metric is bounded by -200% to +200% and the FE metric is bounded by 0% to +200%. We will calculate additional PM model statistical performance metrics to evaluate correlation, variability, error, and bias in the model.

Table 8-2. PM model performance goals and criteria

Metric	Goal	Criteria	Comment
Fractional Bias (FB)	≤± 30%	≤± 60%	PM model performance Goal, considered good PM performance
Fractional Error (FE)	≤ 50%	≤ 75%	PM model performance Criteria, considered average PM performance. Exceeding this level of performance for PM species with significant mass may be cause for concern.

The model performance goals by U.S. EPA and Emery et al. are not used to assign passing or failing grades to model performance, but rather to help interpret the model performance and intercompare across locations, species, time periods and model applications. The model inputs to CAMx vary hourly but tend to represent average conditions that do not account for unusual or extreme conditions. For example, an accident or large event could cause significant increases in congestion and motor vehicle emissions that are not accounted for in the average emissions inputs used in the model.

U.S. EPA compiled and interpreted the model performance from 69 PGM modeling studies in the peer-reviewed literature between 2006 and March 2012 and developed recommendations on what should be reported in a model performance evaluation (Simon, et al., 2012). Although these recommendations are not official U.S. EPA guidance, they are useful and LADCO will refer to them in our model performance evaluation:

- PGM MPE studies should at a minimum report the Mean Bias (MB) and Error (ME or RMSE), Normalized Mean Bias (NMB) and Error (NME), and/or Fractional Bias (FB) and Error (FE). Both the MNB and FB are symmetric around zero with the FB bounded by -200% to +200%.
- Use of the Mean Normalized Bias (MNB) and Gross Error (MNGE) is not encouraged because they are skewed toward low observed concentrations and can be misinterpreted due to the lack of symmetry around zero.

  Given this recommendation the MNB/MNGE will just be calculated for O_3 using an appropriate observed O_3 cut-off concentration (LADCO will use 60 ppb).
- The model evaluation statistics should be calculated for the highest temporal resolution available and for important regulatory averaging times (e.g., daily maximum 8-hour O_3).
- It is important to report processing steps in the model evaluation and how the predicted and observed data were paired and whether data are spatially/temporally averaged before the statistics are calculated.
- Predicted values should be taken from the grid cell that contains the monitoring site, although bilinear interpolation to the monitoring site point can be used for higher resolution modeling (< 12 km).
- $PM_{2.5}$ should also be evaluated separately for each major component species (e.g., SO_4, NO_3, NH_4, EC, OC, and OA).
- Evaluation should be performed for subsets of the data including, high observed concentrations (e.g., O_3 > 60 ppb), by subregions and by season or month.
- Evaluation should include more than just O_3 and $PM_{2.5}$, such as SO_2, NO_2 and CO.
- Spatial displays should be used in the model evaluation to evaluate model predictions away from the monitoring sites. Time series of predicted and observed concentrations at a monitoring site should also be used.
- It is necessary to understand measurement artifacts to make meaningful interpretation of the model performance evaluation.

We will incorporate the recommendations of Simon, Baker and Philips (2012) and Emery et al. (2017) into the LADCO CAMx model performance evaluation.

The LADCO evaluation products will include qualitative and quantitative evaluation for the following model output species:

- Maximum daily 1-hour and maximum daily 8-hour average (MDA8) O_3, including MDA8 with a 60 ppb threshold
- Carbon monoxide, nitrogen dioxide, oxides of nitrogen, sulfur dioxide (SO_2), volatile organic compounds (VOCs) and ammonia (NH_3)
- Total $PM_{2.5}$, elemental carbon, organic carbon, sulfate, nitrate, and ammonium

Table 8-3. Definition of model performance evaluation statistical measures used to evaluate the CTMs.

Statistical Measure	Mathematical Expression	Notes
Accuracy of paired peak (Ap)	$\frac{P - O_{peak}}{O_{peak}}$	Comparison of the peak observed value (O_{peak}) with the predicted value at same time and location
Coefficient of determination (r2)	$1 - \frac{\sum_{i=1}^{N}(O_i - P_i)^2}{\sum_{i=1}^{N}(O_i - \bar{O})^2}$	Pi = prediction at time and location i; Oi = observation at time and location i; $\overline{P}$ = arithmetic average of Pi, i=1,2,…, N; $\overline{O}$ = arithmetic average of Oi, i=1,2,…,N
Normalized Mean Error (NME)	$\frac{\sum_{i=1}^{N}\lvert P_i - O_i\rvert}{\sum_{i=1}^{N} O_i}$	Reported as %
Root Mean Square Error (RMSE)	$\left[\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2\right]^{1/2}$	Reported as %
Fractional Gross Error (FE)	$\frac{2}{N}\sum_{i=1}^{N}\left\lvert\frac{P_i - O_i}{P_i + O_i}\right\rvert$	Reported as % and bounded by 0% to 200%
Mean Absolute Gross Error (MAGE)	$\frac{1}{N}\sum_{i=1}^{N}\lvert P_i - O_i\rvert$	Reported as concentration (e.g., µg/m^3)
Mean Normalized Gross Error (MNGE)	$\frac{1}{N}\sum_{i=1}^{N}\frac{\lvert P_i - O_i\rvert}{O_i}$	Reported as %
Mean Bias (MB)	$\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)$	Reported as concentration (e.g., µg/m^3)
Mean Normalized Bias (MNB)	$\frac{1}{N}\sum_{i=1}^{N}\frac{(P_i - O_i)}{O_i}$	Reported as %
Mean Fractionalized Bias (Fractional Bias, FB)	$\frac{2}{N}\sum_{i=1}^{N}\left(\frac{P_i - O_i}{P_i + O_i}\right)$	Reported as %, bounded by -200% to +200%
Normalized Mean Bias (NMB)	$\frac{\sum_{i=1}^{N}(P_i - O_i)}{\sum_{i=1}^{N} O_i}$	Reported as %
Bias Factor (BF)	$\frac{1}{N}\sum_{i=1}^{N}\left(\frac{P_i}{O_i}\right)$	Reported as BF:1 or 1: BF or in fractional notation (BF/1 or 1/BF).

8.4 Subregional Evaluation of Model Performance

The evaluation of the CAMx 12-km and 4-km base case simulations will focus on a monthly, quarterly, and annual model performance at monitors in each of the six LADCO states. We will also examine summer season high O_3 and $PM_{2.5}$ episodes and winter season high $PM_{2.5}$ episodes in different parts of the region to determine how well the model performs during observed pollution events in 2022.

8.5 Example Model Performance Displays

Below are several examples of model performance displays that will be considered in the LADCO model performance evaluation. We find these visual comparisons of modeled and observed data provide a much better way to convey the model performance than tabular summaries of statistical performance metrics.

8.5.1 Model Evaluation Tools

There are several model performance evaluation tools that may be used in the model evaluation, including the following:

- **VERDI and NCL**: The Visualization Environment for Rich Data Interpretation (VERDI) is a visualization tool specifically designed to visualize photochemical grid model output. It can run on Linux, Windows, or MacOS environments, and it can be used while the photochemical grid model is running or has recently been completed. It is primarily used for spatial maps where modeled tile plots can be displayed with superimposed observations. VERDI can also generate scatter and time series plots. The NCAR Command Language (NCL) is an open-source, Linux command line tool for scientific data visualization. It supports many of the data formats that are used in the LADCO air quality modeling platform, including WRF netCDF, binary, and ASCII.
- **AMET**: The Atmospheric Model Evaluation Tool (AMET) was developed by U.S. EPA and consists of MySQL and R scripts for generating bi-variate model evaluation statistics and graphics. AMET will be used extensively for the LADCO 2022 model performance evaluation of CAMx.

In the following sections, we present examples of model performance evaluation graphics using the above tools like we will use in the WRF, SMOKE, and CAMx model performance evaluation. Because there is redundancy in the some of the displays generated by the different evaluation tools, not all tools will be applied to generate all the different types of graphics.

8.5.2 Time Series Plots

Time series of predicted and observed concentrations are a staple of any model performance evaluation as it allows the user to directly assess how the model is reproducing the time evolution of the observations at different sites. Figure 8-5 displays an example predicted and observed hourly time series comparison for 1-hour average O_3 concentrations at all a single site in Cook County, IL during June 2016 using AMET. The AMET timeseries displays multiple model simulation results to observations in the top panel and the model bias for each hour in the bottom panel.

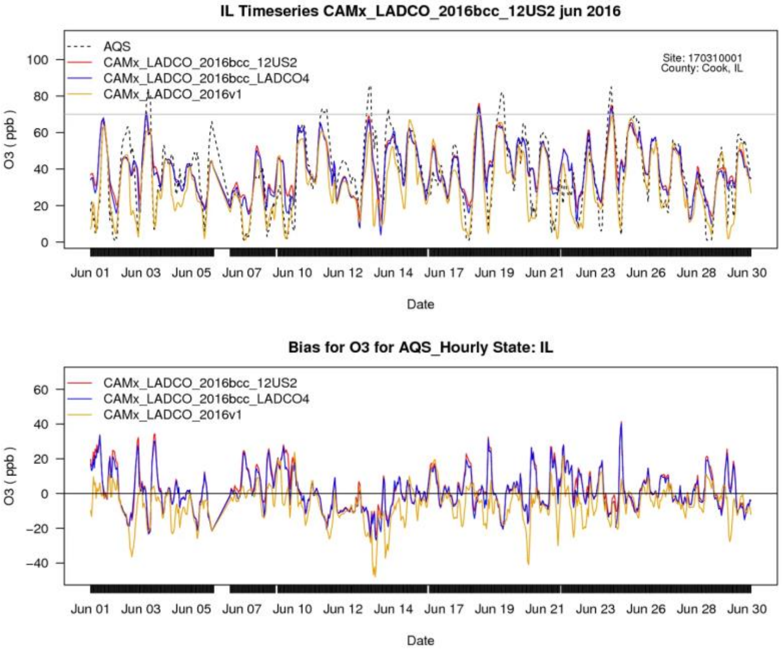

Figure 8-5. Example AMET timeseries plot of June 2016 hourly ozone at a site in Cook County, Illinois.

8.5.3 Box and Whisker of Model Performance Statistics

Figure 8-6 displays monthly average MDA8 O_3 model performance statistics for AQS sites in Michigan for April – September 2016. The box and whisker plots show the observed and model median concentrations as symbols connected by lines (blue for CAMx and black for observations), the 25th and 75th percentile concentrations as the bottom and top of each box, and the 5th and 95th percentile concentrations as the bottom and top of each whisker. Each figure compares CAMx and observations on all days, and only on days with MDA8 O_3 > 60 ppb. In a single plot one can assess how often the model achieves performance goals and whether it tends to have an overall under- or over-prediction bias.

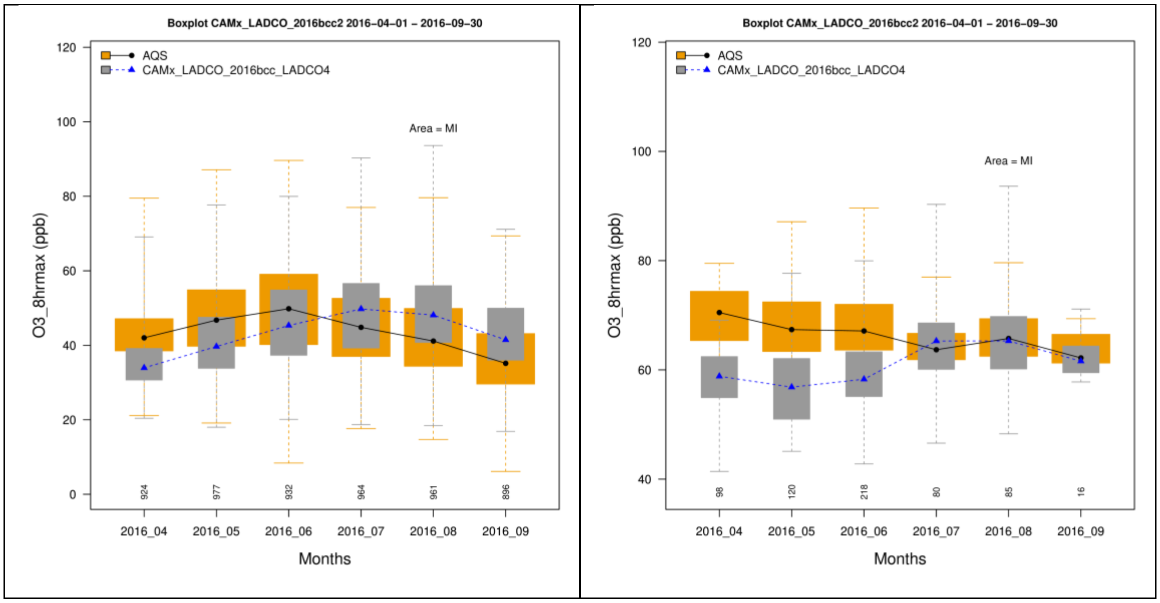

Figure 8-6. 2016 monthly MDA8 O_3 box and whisker plots comparing CAMx with AQS monitors for sites in MI; all days (left) and days with obs > 60 ppb (right)

8.5.4 Kelly Plot

Figure 8-7 is an example of a Kelly plot which shows monthly average results for all monitors in a state across multiple simulations. This example plot compares monthly, state averaged NMB for MDA8 O_3 days > 60 ppb across four CAMx simulations.

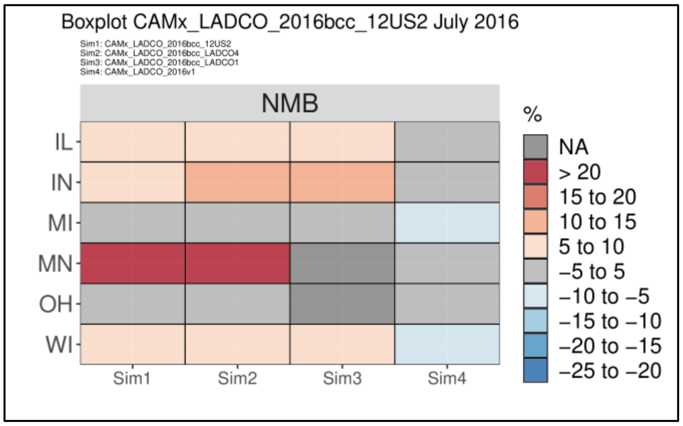

Figure 8-7. July 2016 MDA8 O_3 normalized mean bias state summary plot on days with observed values > 60 ppb

8.5.5 Spatial Plots of Model Performance

Examples of spatial displays of modeling results are presented in Figure 8-8. The left panel compares the predicted 8-hour average O_3 concentrations (the tile plot) with superimposed observations using the same color scale. When the observed symbols are the same color as the background spatial distribution of the model predictions, then the predictions and observations agree with each other. The right panel in Figure 8-8 shows the July 2018 monthly mean normalized bias in O_3 at monitor locations throughout the domain.

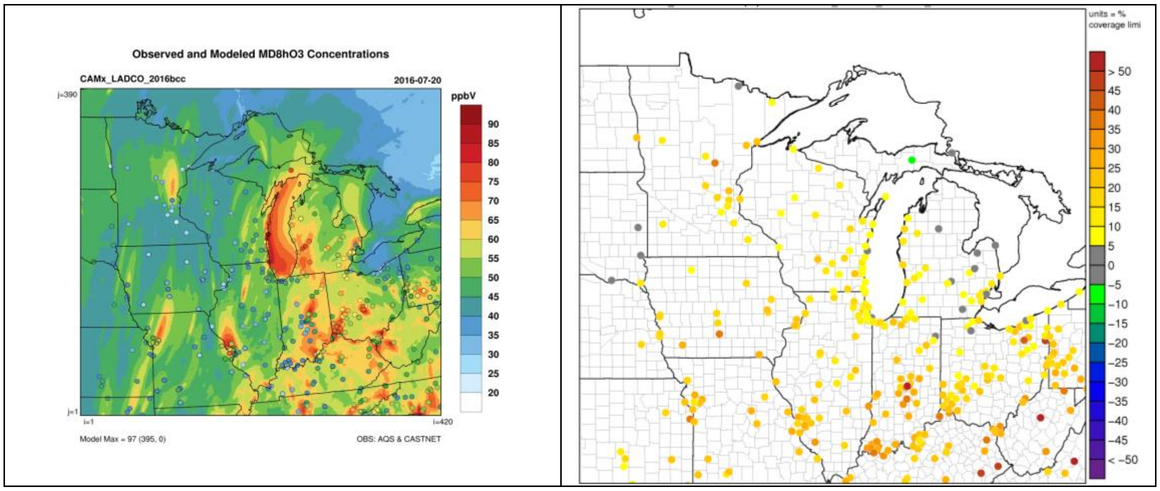

Figure 8-8. Example spatial distribution model performance evaluation displays showing CAMx 4-km daily max MDA O3 performance on July 20, 2016 using observational overlays (left) and July 2016 monthly normalized mean bias for MDA8 O_3 at different monitors using AMET (right)

8.6 Summary of Model Performance

LADCO will conduct a model performance evaluation of the LADCO CAMx 12 km and 4 km 2022 base case simulations for O_3, O_3 precursors, $PM_{2.5}$ and speciated $PM_{2.5}$ concentrations over the LADCO region. This will be followed by sub-regional evaluation of the 4 km modeling results, focusing on time periods and locations with NAAQS compliance issues in 2022.

9 ATTAINMENT DEMONSTRATION PROCEDURES

LADCO will follow the U.S. EPA Modeling Guidance for Demonstrating Air Quality Goals for Ozone, $PM_{2.5}$, and Regional Haze (U.S. EPA, 2018a) to calculate future ozone and $PM_{2.5}$ conditions. As we will use a base year of 2022, we will estimate the base year design values using surface observations for the years 2020-2024 ($DV_{2020\text{-}2024}$). LADCO will use version 2.1 of the Software for Modeled Attainment Test Community Edition (SMAT-CE)[9] to calculate the future year design values at surface monitors according to the SMAT-CE User's Guide (U.S. EPA, 2022). The following sections describe the approaches that LADCO will use for calculating future year O_3 and $PM_{2.5}$ Design Values.

9.1 Future Year O_3 Design Values and Attainment Testing

SMAT-CE will be used to calculate O_3 design values in 2026 and 2032 as projected from the LADCO 2022 base year modeling. We will configure SMAT-CE to use the average O_3 concentration in a 3x3 matrix around each monitor across the 10 highest modeled days, per the U.S. EPA Guidance (2018).

Using the 2026 future year as an example, SMAT-CE uses a four-step process to estimate 2026 Future Design Values (DVF_{2026}) for O_3:

1. Use surface observations to calculate the 2022 base year design values (DVB_{2022}) for each monitor:

The O_3 design value is a three-year average of the 4th highest observed MDA8 ($MDA8_4$) in the three years leading up to the base year:

$$DVB_{2022} = (MDA8_{4,2020} + MDA8_{4,2021} + MDA8_{4,2022})/3$$

2. Calculate the weighted 5-year average of the observed DVBs centered on the base year (2022):

$$DV_{2020\text{-}2024} = (DVB_{2022} + DVB_{2023} + DVB_{2024})/3$$

3. Calculate relative response factor (RRF) for each monitor

Relative response factors are calculated from the CAMx base and future year simulations. First you find the ten days with the highest base year (2022) modeled MDA8 from within a 3x3 matrix of grid cells surrounding each monitor. At least 5 days with modeled MDA8 >= 60 ppb are needed to retain the monitor for the future year DV calculation; if this criterion is not met the monitor is dropped from the DVF calculations. However, due to known issues with model underprediction across the region, LADCO will evaluate dropped monitors on a case-by-case basis, as allowed under EPA's modeling guidance, to ensure the exclusions are reasonable and do not include key O_3 monitors or nonattainment areas.

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[9] https://www.epa.gov/scram/photochemical-modeling-tools

Next, calculate the average MDA8 for the base and future years from the maximum of the values in the 3x3 matrix in each of the selected base year top 10 modeled days. The MDA8 values in the base and future year CAMx simulations are sampled from the same grid cells and days established from the base year results (i.e., they're paired in space and time).

Finally, calculate the RRF as the ratio of the future to base year 10-day averaged MDA8 for each monitor:

$$RRF_{2026} = MDA8_{2026,avg}/MDA8_{2022,avg}$$

4. Calculate DVF_{2026} for each monitor

$$DVF_{2026} = RRF_{2026} * DV_{2020\text{-}2024}$$

The O_3 attainment test compares the DVF_{2026} at each monitor to the O_3 NAAQS to determine if the site is projected to be in attainment or maintenance of the standard. Attainment is determined by truncating DVF_{2026} to an integer and comparing it to the standard. For example, a calculated DVF_{2026} of 70.8 ppbV will be truncated to 70 ppbV, which would pass the attainment test for an O_3 NAAQS of 70 ppbV. Sites with truncated future year DVs greater than or equal to 71 ppbV would fail the attainment test and require additional evidence of emissions reductions to demonstrate that they would meet the NAAQS by the attainment deadline.

If the LADCO future year modeling with on-the-books emissions control programs does not demonstrate attainment of the O_3 NAAQS for all the monitors in the LADCO region, we will work with our member states to design modeling scenarios to investigate alternative emissions reduction scenarios. These alternative modeling scenarios may include:

- Brute force emissions sensitivities in which O_3 precursor emissions (NOx and VOC) are reduced across all anthropogenic sectors;
- Targeted inventory sector emissions reductions (e.g., reduce onroad mobile NOx by 25%);
- Alternative emissions control program scenarios (e.g., impacts of the Cleaner Trucks Initiative);
- Numerical emissions sensitivities (e.g., Direct Decoupled Method) to develop isopleths for NOx/VOC chemical production for nonattainment areas

EPA (2017) clarified that maintenance receptors for O_3 are monitors that are at risk of being nonattainment based on the results from attainment demonstration modeling. U.S. EPA identified the following conditions for which a monitor would be in maintenance of the NAAQS:

- Monitoring sites with current measured values below the NAAQS and average and maximum DVFs exceeding the NAAQS;
- Monitoring sites with average DVFs below the NAAQS but with maximum DVFs exceeding the NAAQS;

- All nonattainment receptors

Following this guidance, U.S. EPA (2018d) presented a series of flexibilities that states may consider when assessing interstate transport. One of the options included in this memo was how to identify maintenance receptors. As the U.S. EPA (2018d) memo creates opportunities for novel approaches to assess maintenance, LADCO will consult with our states and correspond with our U.S. EPA modeling advisors to determine best practices for identifying O_3 maintenance monitors. We will document the methods used to identify nonattainment and maintenance monitors in technical support documentation of our modeling results.

9.2 Future Year Annual $PM_{2.5}$ Design Values and Attainment Testing

SMAT-CE will be used to calculate annual $PM_{2.5}$ design values in 2026 and 2032 as projected from the LADCO 2022 base year modeling. As noted by U.S. EPA (2018), "[b]ecause ambient $PM_{2.5}$ often consists of multiple PM species, the modeled attainment test for $PM_{2.5}$ utilizes both $PM_{2.5}$ and individual $PM_{2.5}$ component species. A separate RRF and a separate concentration representing the base period is calculated for each $PM_{2.5}$ species."

Using the 2032 future year as an example, SMAT-CE uses a four-step process to estimate 2032 annual average $PM_{2.5}$:

1. Compute observed 5-year weighted average quarterly mean $PM_{2.5}$ and quarterly mean composition centered on 2022 for each federal reference method (FRM) monitor.

   First calculate the three-year mean of the 24-hour average $PM_{2.5}$ at each FRM monitor by quarter, e.g., for quarter 1 (January-March):

   $$PM2.5_{2020\text{-}2022,Q1} = ([PM2.5_{2020,Q1}] + [PM2.5_{2021,Q1}] + [PM2.5_{2022,Q1}])/3$$

   Then create the 5-year weighted average centered on 2022 for each quarter, e.g., for quarter 1:

   $$PM2.5_{2020\text{-}2024,Q1} = (PM2.5_{2020\text{-}2022,Q1} + PM2.5_{2021\text{-}2023,Q1} + PM2.5_{2022\text{-}2024,Q1})/3$$

   Next use available observed speciated federal equivalence method (FEM) $PM_{2.5}$ data near the FRM sites to calculate composition at each FRM monitor. EPA (2018) describes the details of how to impose composition on FRM data to calculate quarterly average $PM_{2.5}$ species fractions at each monitor.

   Repeat these procedures for each $PM_{2.5}$ site and quarter to estimate the base year ambient $PM_{2.5}$ species concentrations (composition) to use in the annual $PM_{2.5}$ NAAQS attainment test.

2. Calculate relative response factors (RRF) for the individual $PM_{2.5}$ components by monitor and quarter.

   Relative response factors are calculated from the CAMx base and future year simulations. First compute 3x3 CAMx grid cell matrix, quarterly averages from within a 3x3 matrix of grid cells surrounding each monitor for the 2022 and 2032 simulations. Compute the matrix quarterly average $PM_{2.5}$ concentrations for SO_4, NO_3, OA, EC, soil, and other primary $PM_{2.5}$ (OPP).

Finally, calculate quarterly RRFs for each $PM_{2.5}$ component as the ratio of the future to base year matrix quarterly average concentrations for each monitor:

$$RRF_{2032\ Q1,SO4} = SO4_{2032,Q1} / SO4_{2022,\ Q1}$$

$$RRF_{2032\ Q1,NO3} = NO3_{2032,Q1} / NO3_{2022,\ Q1}$$

$$RRF_{2032\ Q1,OA} = OA_{2032,Q1} / OA_{2022,\ Q1}$$

$$RRF_{2032\ Q1,EC} = EC_{2032,Q1} / EC_{2022,\ Q1}$$

$$RRF_{2032\ Q1,soil} = Soil_{2032,Q1} / Soil_{2022,\ Q1}$$

$$RRF_{2032\ Q1,OPP} = OPP_{2032,Q1} / OPP_{2022,\ Q1}$$

Repeat these procedures for each $PM_{2.5}$ site and quarter to estimate the $PM_{2.5}$ species RRFs to use in the annual $PM_{2.5}$ NAAQS attainment test.

3. Calculate future year $PM_{2.5}$ component concentrations at each FRM monitor

For each $PM_{2.5}$ component, multiply the weighted 5-year average concentrations by the RRF for each species and quarter. For example, for 2032:

$$SO4_{2032,Q1} = RRF_{2032\ Q1,SO4} * SO4_{2020\text{-}2024,Q1}$$

$$NO3_{2032,Q1} = RRF_{2032\ Q1,NO3} * NO3_{2020\text{-}2024,Q1}$$

$$OA_{2032,Q1} = RRF_{2032\ Q1,OA} * OA_{2020\text{-}2024,Q1}$$

$$EC_{2032,Q1} = RRF_{2032\ Q1,EC} * EC_{2020\text{-}2024,Q1}$$

$$OPP_{2032,Q1} = RRF_{2032\ Q1,OPP} * OPP_{2020\text{-}2024,Q1}$$

Repeat these procedures for each $PM_{2.5}$ site and quarter to estimate 2032 $PM_{2.5}$ component concentrations.

4. Calculate the future year annual average $PM_{2.5}$ concentration for the attainment test.

Sum the speciated components for each quarter to estimate the future year quarterly average $PM_{2.5}$ concentrations. Refer to EPA (2018) for important details about the calculations for ammonium, particle bound water, and blank mass in the measurements.

$$PM2.5_{2032,\ Q1} = SO4_{2032,Q1} + NO3_{2032,Q1} + OA_{2032,Q1} + EC_{2032,Q1} + OPP_{2032,Q1} + Water + Blank\ Mass$$

Finally, sum the quarterly average future year $PM_{2.5}$ concentrations to estimate the future year annual average $PM_{2.5}$:

$$PM2.5_{2032} = PM2.5_{2032,\ Q1} + PM2.5_{2032,\ Q2} + PM2.5_{2032,\ Q3} + PM2.5_{2032,\ Q4}$$

10 DOCUMENTATION AND SCHEDULE

LADCO will use this protocol to guide our implementation of a 2022-based air quality modeling platform. As the modeling progresses there will likely be changes to the model configuration, data files, or model applications that differ from the plan presented in this protocol. LADCO will document changes to this protocol in the Protocol Change Log in Appendix A.

LADCO will document the results of the 2022-based modeling in a Technical Support Document (TSD). The TSD will describe the final modeling configuration, details on the model inputs/outputs, evaluation of model performance, and procedures for post-processing the model outputs.

Table 10-1 presents the project schedule for generating a TSD to support 2015 O_3 NAAQS serious area attainment demonstrations in the LADCO member states.

Table 10-1. LADCO 2022 modeling project schedule

Date	Milestone
January 2025	Draft and final modeling protocol
January 2025	2022v1 CAMx-ready emissions completed
March 2025	2022 CAMx simulation completed
March 2025	2026v1 CAMx-ready emissions completed
May 2025	2026 CAMx simulation completed
June 2025	2032v1 CAMx-ready emissions completed
June 2025	2015 O3 NAAQS Draft TSD
July 2025	2015 O3 NAAQS Final TSD
August 2025	2032 CAMx simulation completed

11 REFERENCES

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