Southern New Mexico Ozone Study
Work Plan for the 2011 Modeling Year

Prepared by:

Z. Adelman and J. Bowden
University of North Carolina
Institute for the Environment
Chapel Hill, NC 27599-6116

R. Morris and S. Kemball-Cook
Ramboll Environ US Corporation
773 San Marin Drive, Suite 2115
Novato, California, 94945

October 28, 2015

UNC INSTITUTE FOR THE ENVIRONMENT

RAMBOLL ENVIRON

Page Left Intentionally Blank

Table of Contents

Table of Contents i
List of Figures ii
List of Tables ii
1. Introduction 1
1.1. Project Background 1
1.2. Overview of the SNMOS 2011 Modeling Approach 2
1.3. Organization of the Modeling Plan 3
1.4. Project Participants 4
2. Model Selection 5
2.1. Justification and Overview of Selected Models 5
2.1.1. Meteorological Model 5
2.1.2. Emissions Processing Systems 6
2.1.3. Photochemical Grid Model 9
3. Episode Selection 10
3.1. Episode Selection Criteria 11
3.1.1. Primary Episode Selection Criteria 11
3.1.2. Secondary Criteria 11
3.2. Episode Selection Results 11
4. Domain Selection 12
4.1. Horizontal Modeling Domain 12
4.2. Vertical Domain Structure 16
5. Modeling Specifications 18
5.1. Meteorological Modeling 18
5.1.1. Model Selection 20
5.1.2. Domain Definitions 21
5.1.3. WRF Configuration Specifications 21
5.1.4. Application Methodology 23
5.1.5. Evaluation Approach 23
5.2. Emission Modeling 23
5.3. Photochemical Modeling 32
6. CAMx Model Performance Evaluation 37
6.1. Available Aerometric Data for the model Evaluation 38
6.2. Model Performance Statistics, Goals and Criteria 39
7. Acronyms 42
8. References 44

List of Figures

Figure 1. SNMOS WRF modeling domains. 14

Figure 2. SNMOS 2011 CAMx 12/4-km modeling domains and the WAQS (identical to 3SAQS) 12 km grid that will supply BCs to the SNMOS 12 km grid. 15

Figure 3. SNMOS 2025 CAMx source apportionment 36/12/4-km modeling domains. 16

Figure 4. Air quality monitors in New Mexico and the surrounding area 38

List of Tables

Table 1. Daily maximum 8-hour average ozone measurements from 2011-2014 at AQS sites in Doña Ana County, NM 1

Table 2. Project contacts for the SNMOS. 4

Table 3. SNMOS WRF domain projection and grid parameters 14

Table 4. SNMOS CAMx domain projection and grid parameters 15

Table 5. 33 vertical layer interface definition for WRF and CAMx simulations. 17

Table 6. Base configuration for the SNMOS WRF sensitivity modeling 20

Table 7. SNMOS emissions inventory sectors 24

Table 8. SNMOS emissions processing sectors 31

Table 9. SNMOS CAMx version 6.20 configuration 35

Table 10. Ozone and PM model performance goals and criteria 39

1. Introduction

1.1. Project Background

Doña Ana County in Southern New Mexico experiences some of the highest observed ground-level ozone concentrations in the state. The Sunland Park Ozone Nonattainment Area (NAA) which lies within Doña Ana County was designated as marginal nonattainment for the 1-hour ozone standard on June 12, 1995 (60 FR 30789). With the revocation of the 1-hour ozone standard in 2004, the Sunland Park NAA was designated a maintenance area for 8-hour ozone (NMED, 2007). Lowering of the 8-hour ozone standard by EPA in 2008 to 0.75 ppm (75 ppb) and again in 2015 to 0.70 ppm (70 ppb) will likely lead to the Sunland Park NAA receiving a nonattainment designation for 8-hour ozone. In addition, the New Mexico Air Quality Control Act (NMAQCA) requires the New Mexico Environment Department (NMED) to develop a plan for reducing ozone levels in areas that are within 95% of the ozone standard (NMSA 1978, § 74-2-5.3). Table 1 shows the 1st through 4th highest daily maximum 8-hour average ozone (MDA8) concentrations measured from 2011 to 2014 at the AQS monitors in Doña Ana County. This table shows that all but a handful of the measurements at these monitors exceeded either the 2015 NAAQS for ozone (orange) or the NMAQCA 95% threshold (yellow).

Table 1. Daily maximum 8-hour average ozone measurements from 2011-2014 at AQS sites in Doña Ana County, NM

Station	1st Highest		2nd Highest		3rd Highest		4th Hightest	
	Date	ppmV	Date	ppmV	Date	ppmV	Date	ppmV
La Union	5/24/2011	0.064	6/22/2011	0.064	7/28/2011	0.064	4/26/2011	0.063
SPCY	6/22/2011	0.078	6/4/2011	0.076	7/28/2011	0.068	6/27/2011	0.067
Chaparral	8/2/2011	0.074	5/24/2011	0.073	5/25/2011	0.071	6/22/2011	0.07
Desert V	6/4/2011	0.084	6/22/2011	0.081	8/27/2011	0.073	7/28/2011	0.072
Sta Teresa	6/22/2011	0.078	5/24/2011	0.074	4/26/2011	0.07	6/27/2011	0.07
Solano	5/24/2011	0.068	5/25/2011	0.068	8/6/2011	0.068	8/27/2011	0.067
La Union	8/31/2012	0.079	7/13/2012	0.078	6/28/2012	0.075	7/14/2012	0.074
SPCY	8/31/2012	0.078	7/13/2012	0.076	7/12/2012	0.075	6/28/2012	0.073
Chaparral	6/2/2012	0.075	6/1/2012	0.07	7/13/2012	0.069	6/3/2012	0.067
Desert V	7/13/2012	0.077	8/31/2012	0.077	7/12/2012	0.076	6/28/2012	0.075
Sta Teresa	8/31/2012	0.083	7/13/2012	0.08	7/12/2012	0.078	9/1/2012	0.077
Solano	5/16/2012	0.069	6/3/2012	0.068	7/13/2012	0.067	6/2/2012	0.066
La Union	8/17/2013	0.066	8/16/2013	0.065	8/21/2013	0.065	8/4/2013	0.064
SPCY	7/3/2013	0.068	6/11/2013	0.063	6/9/2013	0.063	8/17/2013	0.062
Chaparral	5/24/2013	0.074	6/15/2013	0.074	7/3/2013	0.071	7/5/2013	0.07
Desert V	7/3/2013	0.076	8/16/2013	0.072	7/27/2013	0.072	6/9/2013	0.071
Sta Teresa	7/27/2013	0.089	7/3/2013	0.081	7/25/2013	0.081	7/7/2013	0.08
Solano	7/31/2013	0.066	7/27/2013	0.065	7/16/2013	0.065	5/20/2013	0.064
La Union	6/10/2014	0.07	5/29/2014	0.07	8/18/2014	0.068	5/28/2014	0.066
SPCY	6/10/2014	0.073	5/29/2014	0.068	8/30/2014	0.068	7/22/2014	0.068
Chaparral	8/6/2014	0.075	6/10/2014	0.071	7/18/2014	0.069	5/29/2014	0.068
Desert V	6/10/2014	0.077	5/29/2014	0.074	7/15/2014	0.073	5/28/2014	0.072

Sta Teresa	7/15/2014	0.071	8/18/2014	0.07	7/31/2014	0.069	6/10/2014	0.067
Solano	6/10/2014	0.072	6/7/2014	0.069	5/29/2014	0.068	6/9/2014	0.067

The statutory requirements of both the NAAQS and the NMAQCA include the development of a plan to control the emissions of sources pursuant to attainment and maintenance of the NAAQS. In the case of a NAAQS NAA State Implementation Plan (SIP), air quality modeling is required to identify the causes of high pollution and to propose emissions control strategies that will bring the area into attainment. The Southern New Mexico Ozone Study (SNMOS) will study the factors contributing to high ozone in Doña Ana County and investigate future emissions scenarios that will produce NAAQS attainment. The SNMOS is a collaborative project between NMED, the Western Regional Air Partnership (WRAP), the Western Air Resources Council (WESTAR), Ramboll Environ, Corporation (RE), and the University of North Carolina Institute for the Environment (UNC-IE). This Study builds off of the Western Air Quality Study (WAQS), a cooperative project that is intended to facilitate air resource analyses for federal and state agencies in the intermountain western U.S. toward improved information for the public and stakeholders as a part of air quality planning. The Intermountain West Data Warehouse (IWDW) at the Cooperative Institute for Research in the Atmosphere (CIRA) at Colorado State University is the source for the regional air quality modeling data and software resources from the WAQS. The SNMOS will leverage the WAQS 2011 version B (WAQS_2011b) modeling platform to conduct base and future year air quality modeling for Doña Ana County.

1.2. Overview of the SNMOS 2011 Modeling Approach

The SNMOS modeling platform (SNMOS_2011a) will be derived from the WAQS_2011b regional modeling platform. A regional modeling platform is the suite of data and software required for conducting a regional-scale air quality modeling study. The procedures for the SNMOS 2011 modeling will follow those performed for the 2011 WAQS with adjustments to the meteorology and modeling domains to optimize the modeling platform for application to southern New Mexico. The SNMOS_2011a modeling platform will include nested 36, 12 and 4-km resolution meteorology modeling domains. The regional air quality modeling will be conducted at 12 and 4 km resolution. The SNMOS 12 and 4-km domains are designed to encompass the meteorology and emissions features that are most important to ground-level ozone formation in southern New Mexico. We will simulate the 2011 ozone season and evaluate the meteorology and air quality model performance against surface and aloft monitors that operated in the modeling domains during the study period. Following the base year model performance evaluation we will use projected emissions data to simulate air quality in the year 2025. Along with future year attainment tests, the future year modeling will include ozone source apportionment modeling of source region and source category contributions to ozone concentrations and ozone design values at ozone monitoring in Doña Ana county (and elsewhere in the region). A summary of the SNMOS 2011 modeling approach is given below, with more details provided in the subsequent chapters of this modeling plan.

- The 2011 ozone season for New Mexico (May 1 – September 30) was selected for the modeling period.
- Year 2011 and 2025 inventories will be used to estimate base and future year emissions.
- The modeling domains will include a 36-km continental U.S. (CONUS36) domain, a 12-km western U.S. (WESTUS12) domain, and a 4-km Southeastern New Mexico

(SNMOS04) domain. The WESTUS12 photochemical modeling domain encompasses regional metropolitan areas and large emissions sources likely to contribute to ozone in Doña Ana County, while the high resolution SNMOS4 domain focuses on Doña Ana County and its immediate vicinity.

- The Weather Research Forecasting (WRF) version 3.7.1 will be used to simulate meteorology data for this study.
- Emissions processing will primarily be conducted using the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system version 3.7 using emissions data from the EPA 2011-based modeling platform (2011v6) version 2 and the WAQS (2011b).
- Photochemical grid modeling (PGM) will be done with the Comprehensive Air-quality Model with extensions (CAMx) version 6.20. The Carbon Bond 6 revision 2 (CB6r2) photochemical mechanism will be used for the SNMOS_2011a modeling.
- For the SNMOS 2011 modeling, hourly boundary conditions (BCs) for the portion of the lateral boundaries of the SNMOS WESTUS12 PGM domain that lies within the larger WAQS WESTUS12 domain will be will be extracted from the WAQS WESTUS12 CAMx results. For the portion of the SNMOS WESTUS12 grid that lies outside the WAQS WESTUS12 grid, we will extract lateral BCs from the WAQS 36-km CONUS CAMx modeling.
- Model evaluation will be conducted for meteorology, ozone, and ozone precursor and product species.
- Diagnostic sensitivity tests will be conducted to determine sensitivity of the PGM model estimates to key parameters and to improve the base year model performance.
- Future year modeling will be used to estimate air quality in 2025 and to conduct attainment tests for Doña Ana County.
- Future year emissions sensitivity modeling will be used to evaluate the impacts of emissions reductions on future attainment of the ozone NAAQS.
- Future year CAMx source apportionment modeling will be used to quantify the source region and source category contributions to ozone concentrations and ozone design values at ozone monitoring in Dona Ana County.

1.3. Organization of the Modeling Plan

This document presents the SNMOS modeling plan for 2011-based meteorology, emissions, and PGM simulations. Although the SNMOS modeling analysis is not currently being performed to fill any particular regulatory requirement, such as a State Implementation Plan (SIP) attainment demonstration, it is being conducted with the same level of technical rigor as a SIP-type analysis.

This SNMOS Modeling Plan has the following sections:

1. Introduction: Presents a summary of the background, purpose and objectives of the study
2. Model Selection: Introduces the models selected for the study
3. Episode Selection: Describes the modeling period for the study
4. Modeling Domain Selection: Presents the modeling domains selected for the study
5. WRF Meteorology: Describes how the meteorological modeling was conducted and the WRF model evaluation
6. Emissions: Describes the emissions input data, how the emissions modeling will be conducted, 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. Acronyms: Definitions of acronyms used in this document
10. References: References cited in the document

1.4. Project Participants

The SNMOS is facilitated and managed by the Western States Air Resources Council (WESTAR). RE and UNC-IE are conducting the meteorology, emissions, and air quality modeling and analysis. Key contacts and their roles in the SNMOS are listed in Table 2

Name	Role	Organization/Contact
Tom Moore	Project Manager	WESTAR c/o CSU/CIRA 1375 Campus Delivery Fort Collins, CO 80523 (970) 491-8837 tmoore@westar.org
Zac Adelman	UNC-IE Lead	University of North Carolina Institute for the Environment 100 Europa Dr., Suite 490, CB 1105 Chapel Hill, NC 27517 (919) 962-8510 zac@unc.edu
Ralph Morris	Ramboll Environ Lead	Ramboll Environ 773 San Marin Drive, Suite 2115 Novato, CA 94998 (415) 899-0708 rmorris@environcorp.com

.

Table 2. Project contacts for the SNMOS.

Name	Role	Organization/Contact
Tom Moore	Project Manager	WESTAR c/o CSU/CIRA 1375 Campus Delivery Fort Collins, CO 80523 (970) 491-8837 tmoore@westar.org
Zac Adelman	UNC-IE Lead	University of North Carolina Institute for the Environment 100 Europa Dr., Suite 490, CB 1105 Chapel Hill, NC 27517 (919) 962-8510 zac@unc.edu
Ralph Morris	Ramboll Environ Lead	Ramboll Environ 773 San Marin Drive, Suite 2115

		Novato, CA 94998 (415) 899-0708 rmorris@environcorp.com

2. Model Selection

This section discusses the meteorology, emissions, and air quality modeling software used for the SNMOS. The modeling software selection methodology follows EPA's guidance for regulatory modeling in support of ozone and $PM_{2.5}$ attainment demonstration modeling and showing reasonable progress with visibility goals (EPA, 2007; EPA, 2014d). EPA recommends that models be selected for regulatory ozone, 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 of these considerations should be examined for each class of models to be used (e.g., emissions, meteorological, and photochemical) in part because EPA no longer recommends a specific model or suite of photochemical models for regulatory application as it did twenty years ago in the first ozone SIP modeling guidance (EPA, 1991). Below we identify the most appropriate candidate models that we believe are best suited to the requirements of the SNMOS, discuss the candidate model attributes and then justify the model selected using the four criteria above. The science configurations recommended for each model in this study are introduced in Chapter 5. Chapter 6 presents the PGM model performance evaluation procedures that we will use to evaluate CAMx.

2.1. Justification and Overview of Selected Models

The SNMOS will be using three general types of models for simulating ozone in the region of Doña Ana County:

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

These are not single models, but rather suites of models or modeling systems that are used to generate PGM meteorological and emissions inputs and simulate air quality.

2.1.1. Meteorological Model

The Weather Research Forecast Model (WRF) is currently the only prognostic meteorological model that is routinely used in the U.S. in photochemical grid modeling studies.

With coordination and support from the National Center for Atmospheric Research (NCAR), the meteorology modeling research community developed WRF, and its predecessor MM5. For many years the MM5 model was widely used by both the meteorological research as well as the air quality modeling community. Starting around the year 2000, the WRF model started to be developed as a technical improvement and replacement to MM5 and today NCAR no longer supports MM5. WRF is a defensible meteorological driver to PGM modeling for the following reasons:

- Technical: WRF is based on recent physics and computing techniques. A large community of users and developers currently supports it.
- 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 is amassing 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: Recent WRF modeling in the Western U.S. has demonstrated that the model can generally simulate the conditions to lead to high ozone formation (UNC and ENVIRON, 2015). With each subsequent WRF application, new features and improvements are made to further improve the performance of the model.

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

WRF version 3.7.1: The non-hydrostatic version of the Advanced Research version of the Weather Research Forecast (WRF-ARW[1]) model (Skamarock et al. 2004; 2005; 2006) is a three-dimensional, limited-area, primitive equation, prognostic model that has been used widely in regional air quality model applications. The basic model has been under continuous development, improvement, testing and open peer-review for more than 10 years and has been used world-wide by hundreds of scientists for a variety of mesoscale studies, including cyclogenesis, polar lows, cold-air damming, coastal fronts, severe thunderstorms, tropical storms, subtropical easterly jets, mesoscale convective complexes, desert mixed layers, urban-scale modeling, air quality studies, frontal weather, lake-effect snows, sea-breezes, orographically induced flows, and operational mesoscale forecasting. 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 the National Center for Atmospheric Research and the National Centers for Environmental Prediction, WRF is maintained and supported as a community model by researchers and practitioners around the globe. The code supports two modes: the Advanced Research WRF (ARW) version and the Non-hydrostatic Mesoscale Model (NMM) version. It is suitable for use in a broad spectrum of applications across scales ranging from hundreds of meters to thousands of kilometers.

WRF-ARW version 3.7.1 will be used for the SNMOS.

2.1.2. Emissions Processing Systems

The following software will be used to prepare emissions inputs for the CAMx PGM used in the 3SAQS.

- Sparse Matrix Operator Kernel Emissions (SMOKE) processor, version 3.7 – software system that prepares emission inventory data for input to a PGM; primary functions include spatial, temporal, and chemical conversion of emission inventory data to the terms required by a PGM
- Model of Emissions of Gases and Aerosols from Nature (MEGAN), version 2.10 (Guenther et al., 2012) – biogenic emissions model; primary function is to estimate gridded gas-phase emissions from plants and soils

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

- WRAP Windblown Dust Model (WRAP-WBD; Mansell et al., 2006) - software to estimate wind-driven dust emissions

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 two emissions processors that are routinely used in the U.S. in photochemical grid modeling studies:

- The Emissions Processing System (EPS); and
- The Sparse Matrix Operator Kernel Emissions (SMOKE) system.

These software systems are considered emissions processors and 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. The EPS system is currently only routinely used by the state of Texas. We have selected SMOKE as the emissions processor for the SNMOS to leverage the EPA NEI and WAQS modeling platforms, which used SMOKE. SMOKE is a reasonable choice of emissions processor for this study for the following reasons:

- Technical: SMOKE is undergoing the most active development and updates of all of the processors listed above. It is updated 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 EPA.
- Performance: SMOKE is designed to be efficient in how it processes large quantities of data. It has been used in countless research and regulatory studies worldwide and is most likely the emissions processor in recently published regional modeling studies that used either the CMAQ or CAMx PGM.
- Public Availability: SMOKE is publicly available and can be downloaded from the Community Modeling and Analysis System Center with no costs or restrictions.
- Demonstrated Success: The Denver 2008 SIP modeling, the Three State Air Quality Study (UNC and ENVIRON, 2013; UNC and ENVIRON, 2014), and the WAQS all used SMOKE for preparing the PGM emissions. While some of the deficiencies in the model performance in all of these studies may be partially traced to flaws in 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.

SMOKEv3.7: The Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system is a set of programs that is used by the U.S. EPA, Regional Planning Organizations (RPOs), 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 (U.S. EPA, 2004).

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 can additionally be used to 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 is designed with flexible QA capabilities to generate standard and custom reports for checking the emissions modeling process. After modeling all of the emissions source categories individually, SMOKE creates two files per day for input into CMAQ and CAMx: (1) an elevated point source file for large stationary sources, and (2) a merged gridded source file of low-level point, mobile, non-road, area, and biogenic emissions. 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 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 temporal and spatial extents of the SMOKE modeling periods are dictated by the input meteorology. 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 that are 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. These rules are explicitly laid out in the SMOKE User's Manual. 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.

In general 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), which is 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, is needed to create 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 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. Details of the data used for the 3SAQS are provided in the next section.

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 mobile sources. MOVES is capable of creating inventories or lookup tables at the national, state, county, or project scales. MOVES was designed by EPA's Office of Transportation and Air Quality (OTAQ) and the current version is MOVES2014 that was released in July 2014. MOVES is principally an emissions modeling system where emissions estimates are simulated from 'first principles' taking 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. MOVES outputs can be input to emissions processing systems such as SMOKE.

MEGAN: The Model of Emissions of Gases and Aerosols in Nature (MEGAN) is a modeling system for estimating the net emission of gases and aerosols from terrestrial ecosystems into the atmosphere (Jiang et al., 2012; Wiedinmyer, Sakulyanontvittaya and Guenther, 2007). Driving variables include landcover, weather, and atmospheric chemical composition. MEGAN is a global model with a base resolution of ~1 km and so is suitable for regional and global models. A FORTRAN code is available for generating emission estimates for the CMAQ and CAMx regional air quality models. Global distributions of landcover variables (Emission Factors, Leaf Area Index, and Plant Functional Types) are available for spatial resolutions ranging from ~ 1 to 100 km and in several formats (e.g., ARCGIS, netcdf). WRAP has recently updated the MEGAN biogenic emissions models using western U.S. data and higher resolution inputs (Sakulyanontvittaya, Yarwood and Guenther, 2012).

2.1.3. Photochemical Grid Model

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

- Community Multiscale Air Quality (CMAQ) modeling system; and
- Comprehensive Air-quality Model with extensions (CAMx).

CMAQ is developed by EPA and CAMx is developed by Ramboll Environ. Both models are publicly available and have adopted the "one-atmosphere" concept treating ozone, $PM_{2.5}$, air toxics, visibility and other air quality issues within a single platform.

- Technical: Both CMAQ and CAMx represent state-of-science one-atmosphere PGMs. Both models were selected for use in the WAQS. CAMx was selected for the SNMOS applications because it supports two-way grid nesting and source apportionment modeling.
- Performance: A peer-review of the CAMx and CMAQ source apportionment algorithms found CAMx to be technically and operationally superior to CMAQ. CAMx also tends to run a little faster than CMAQ.
- Public Availability: CMAQ and CAMx are both publicly available.

- Demonstrated Success: Both CMAQ and CAMx have had many successful model performance applications. CAMx has been applied more frequently in the Rocky Mountain region for NEPA studies and the Denver ozone SIP modeling.

The CAMx and CMAQ models are summarized below.

CAMxv6.20: The Comprehensive Air Quality Model with Extensions (CAMx) 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 (ENVIRON, 2014). 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 ozone, 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. The U.S. EPA has approved the use of CAMx for numerous ozone and PM State Implementation Plans throughout the U.S. and 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.).

CMAQv5.1: EPA's Models-3/Community Multiscale Air Quality (CMAQ) modeling system is also "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 (Byun and Ching, 1999). The CMAQ modeling system was designed to approach air quality as a whole by including state-of-the-science capabilities for modeling multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation. CMAQ was also designed to have multi-scale capabilities so that separate models were not needed for urban and regional scale air quality modeling. The CMAQ modeling system contains three types of modeling components: (a) a meteorological module for the description of atmospheric states and motions, (b) an emission models for man-made and natural emissions that are injected into the atmosphere, and (c) a chemistry-transport modeling system for simulation of the chemical transformation and fate.

CAMx Version 6.20 (March 2015) will be used for the SNMOS modeling for the following reasons:

- To leverage the WAQS CAMx 2011 modeling platform;
- The CAMx source apportionment functions are further developed and better evaluated than the CMAQ source apportionment tools.

3. Episode Selection

EPA's ozone, $PM_{2.5}$ and visibility SIP modeling guidance (EPA, 2007; EPA, 2014) contains recommended procedures for selecting modeling episodes, while also referencing EPA's 1-hour ozone modeling guidance for episode selection (EPA, 1991). This Chapter presents the modeling period selected for performing the SNMOS and the justification and rationale for its selection.

3.1. Episode Selection Criteria

EPA's modeling guidance lists primary criteria for selecting episodes for ozone, $PM_{2.5}$ and visibility SIP modeling along with a set of secondary criteria that should also be considered.

3.1.1. Primary Episode Selection Criteria

EPA's modeling guidance (EPA, 2007; EPA, 2014) identifies four specific criteria to consider when selecting episodes for use in demonstrating attainment of the 8-hour ozone NAAQS:

1. A variety of meteorological conditions should be covered, including the types of meteorological conditions that produce 8-hour ozone exceedances in the western U.S.;
2. Choose episodes having days with monitored 8-hour daily maximum ozone concentrations close to the ozone Design Values;
3. To the extent possible, the modeling data base should include days for which extensive data bases (i.e. beyond routine aerometric and emissions monitoring) are available; and
4. Sufficient days should be available such that relative response factors (RRFs) for ozone projections can be based on several (i.e., > 10) days with at least 5 days being the absolute minimum.

3.1.2. Secondary Criteria

EPA also lists four "other considerations" to bear in mind when choosing potential 8-hour ozone 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.

EPA suggests that modeling an entire summer ozone season for ozone would be a good way to ensure 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 ozone Design Value projections.

3.2. Episode Selection Results

May through August 2011 was selected for the SNMOS modeling because it builds off the WAQS modeling. The selection of this period also satisfies several of the episode selection criteria listed above:

1. Modeling the entire 2011 ozone season will capture a variety of conditions that lead to elevated ozone in southern New Mexico
2. 2011 is also a National Emissions Inventory (NEI) update year and the NEI is an important database required for modeling.
3. The four-month ozone season simulation will assure sufficient days are available to analyze ozone formation and impacts. Simulating the entire season also provides the opportunity to simulate the North American Monsoon season, which strongly influences ozone concentrations in the region.

4. In addition to the WAQS, 2011 is being used for other studies including several BLM Environmental Impact Statements (EISs) and Resource Management Plans (RMPs).
5. Several weekday-weekend cycles are included in the entire ozone season simulation.

The decision to model just the summer ozone season and not the entire year is based on the need to only address ozone and not $PM_{2.5}$, visibility and deposition issues.

4. Domain Selection

This Chapter summarizes the selection and model domain definitions for the SNMOS 2011 photochemical grid modeling (PGM), including the domain coverage, resolution, map projection, and nesting schemes for the high resolution sub-domains. The modeling domains for the WRF meteorological modeling are defined slightly larger than the PGM domains and are given in Chapter 5.

4.1. Horizontal Modeling Domain

The SNMOS modeling domains were selected to facilitate high resolution modeling for sources around Doña Ana County and to enable regional source apportionment modeling among all of the surrounding Western states. The SNMOS meteorology modeling will use 36, 12 and 4-km one-way nested domains. The WRF meteorological model requires use of an odd nesting ratio so the 36/12/4-km domains are using a 3:1 grid-nesting ratio. Consistent will the majority of regional modeling studies over the mid-latitudes, a Lambert Conformal Projection (LCP) centered on 40N and 97W will be used for horizontal modeling domains using the parameters in Table 3.

Figure 1 illustrates the SNMOS WRF domains, which are considerably larger than the CAMx modeling domains. The WRF domains were chosen for the following reasons:

- A 36-km continental U.S. (CONUS36) domain is the same as used by the RPOs (e.g., WRAP) and most other recent modeling studies (e.g., WAQS). It is defined large enough so that the outer boundaries are far away from our primary areas of interest (i.e., western states).
- A 12-km western U.S. (WESTUS12) domain is the same size as the WAQS 12-km domain but shifted south to support the resolution of North American Monsoon features that evolve in the southern portion of the modeling domain.
- A 4-km southern New Mexico (SNMOS04) domain focuses on Doña Ana County.

CAMx modeling of 2011 for the SNMOS will be performed on nested 12/4 km modeling grids focused on Doña Ana County. **Error! Reference source not found.** displays the 12-km WESTUS12 and 4-km SNMOS04 CAMx and emissions processing domains. Table 4 details the CAMx domain parameters. The CAMx and emissions domains for modeling of 2011 were chosen for the following reasons:

- New continental-scale coarse grid modeling is not needed for the SNMOS because we are able to extract BCs for the 12-km domain from the WAQS 2011 CAMx modeling results. The WAQS modeling used the 36-km RPO grid and a 12-km modeling domain that encompassed much of the western U.S. As we're using the same emissions data and CAMx configuration for the SNMOS as were used for the WAQS, there will be

consistency between these simulations enabling the use of the WAQS modeling as BCs for the SNMOS domains.

- The SNMOS WESTUS12 CAMx domain encompasses all of New Mexico, extends west to include the metropolitan area of Phoenix, east to include East Texas, and South to include the Carbon II power plant in Coahuila, Mexico. This facility is a large source of NOx emissions and lies in a region that was sometimes upwind of Doña County on high ozone days during 2011. The SNMOS WESTUS12 domain was designed as a tradeoff between computational efficiency and the need to model transport from sources likely to influence Doña Ana County at 12 km resolution.
- The SNMOS04 4-km Doña Ana County domain focuses on Southern NM and the major source regions in the immediate vicinity, including Ciudad Juarez, Mexico and El Paso, TX.

For the 2025 future year source apportionment modeling, we will use a grid configuration that is different from that of the 2011 modeling, but uses the 36/12/4 km grids described in **Error! Reference source not found.**. We expect that a source apportionment analysis performed on the 2011 model grid configuration would contain a large contribution from the 12 km boundary conditions. In order to understand the role of transport in high ozone in Doña Ana County, it is important to be able to distinguish between contributions to Doña Ana County ozone from regions outside the U.S. and regions within the U.S. Therefore, we will use a nested 36/12/4-km model configuration for the 2025 source apportionment modeling to allow identification of contributions from regions outside the 12 km grid, but within the 36 km grid (e.g. Los Angeles). The 36-km CAMx modeling will use the WAQS 36-km modeling platform and will be therefore be consistent with the WAQS modeling used to supply boundary conditions for the 2011 SNMOS modeling. Therefore, the 2025 source apportionment modeling will be consistent with the 2011 SNMOS modeling. Because running the 36/12/4-km nested source apportionment simulation will require far more computing resources than running a 12/4 simulation, the 2025 source apportionment modeling will focus on periods when Doña Ana County had high 8-hour average ozone in 2011.

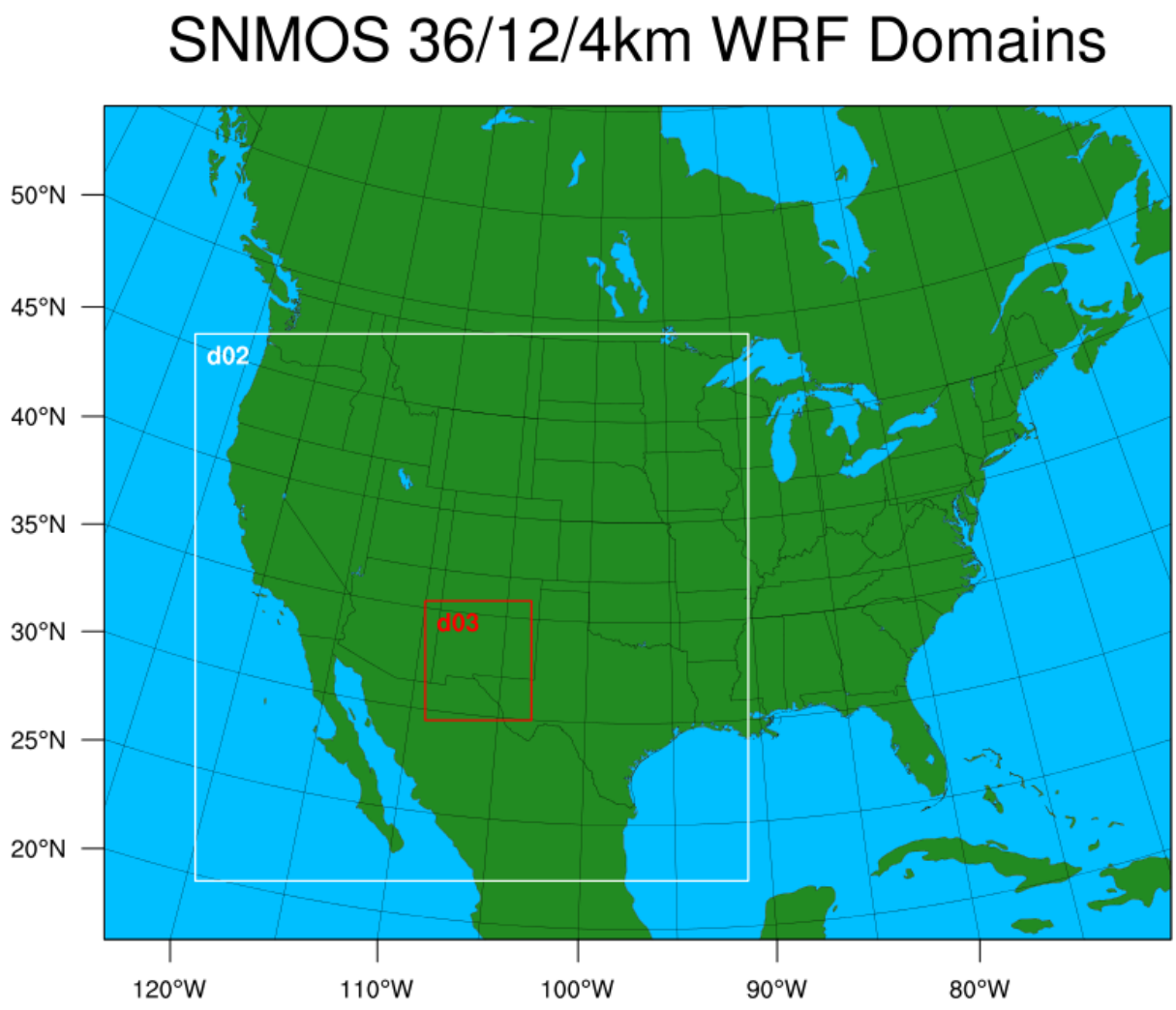

Figure 1. SNMOS WRF modeling domains.

Table 3. SNMOS WRF domain projection and grid parameters

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
dX (km)	d01 = 36, d02 = 12, d03 = 4
dY (km)	d01 = 36, d02 = 12, d03 = 4
X-orig (km)	d01 = -2736, d02 = -2196, d03 = -912
Y-orig (km)	d01 = -2088, d02 = -1728, d03 = -828
# cols	d01 = 165, d02 = 256, d03 = 148
# rows	d01 = 129, d02 = 253, d03 = 166

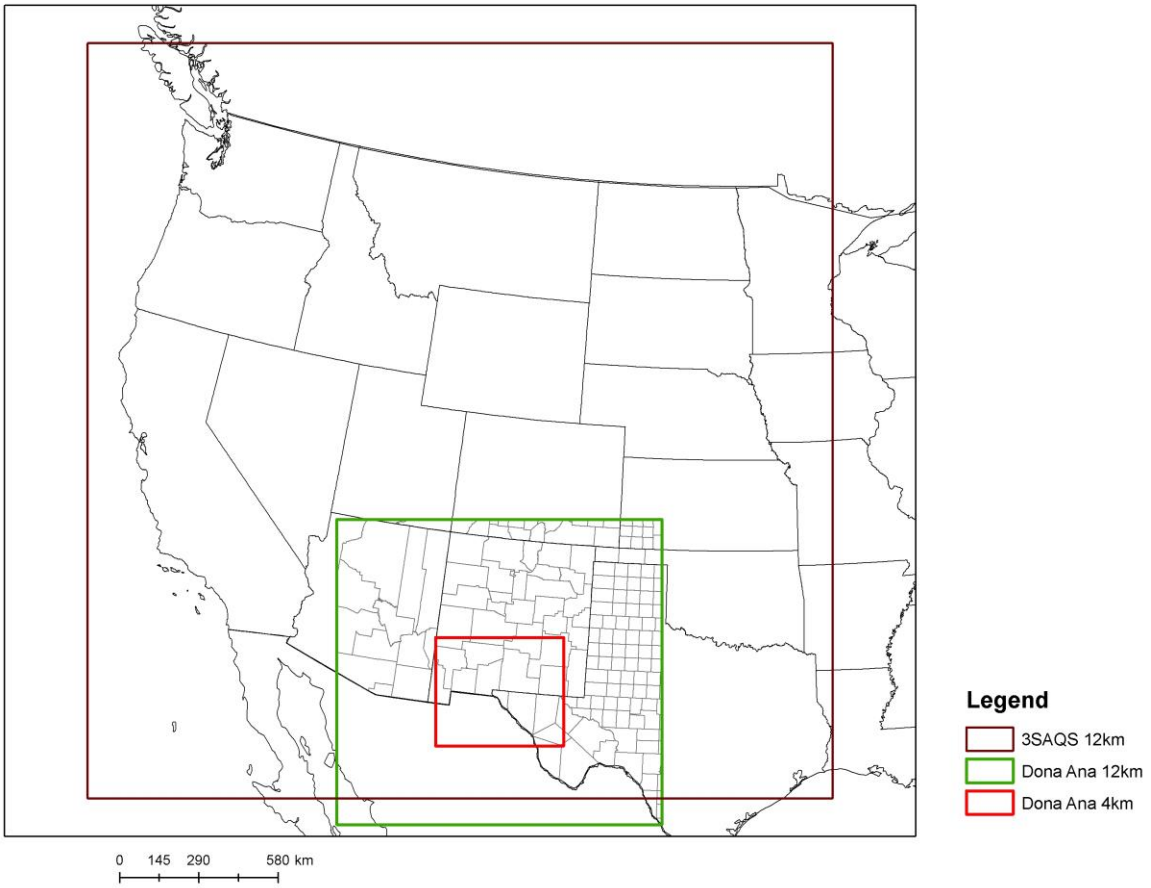

Figure 2. SNMOS 2011 CAMx 12/4-km modeling domains and the WAQS (identical to 3SAQS) 12 km grid that will supply BCs to the SNMOS 12 km grid.

Table 4. SNMOS CAMx domain projection and grid parameters

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
dX (km)	d01 = 36, d02 = 12, d03 = 4
dY (km)	d01 = 36, d02 = 12, d03 = 4
X-orig (km)	d01 = -2736, d02 = -1476, d03 = -1116
Y-orig (km)	d01 = -2088, d02 = -1332, d03 = -1044
# cols	d01 = 148, d02 = 99, d03 = 117
# rows	d01 = 112, d02 = 93, d03 = 99

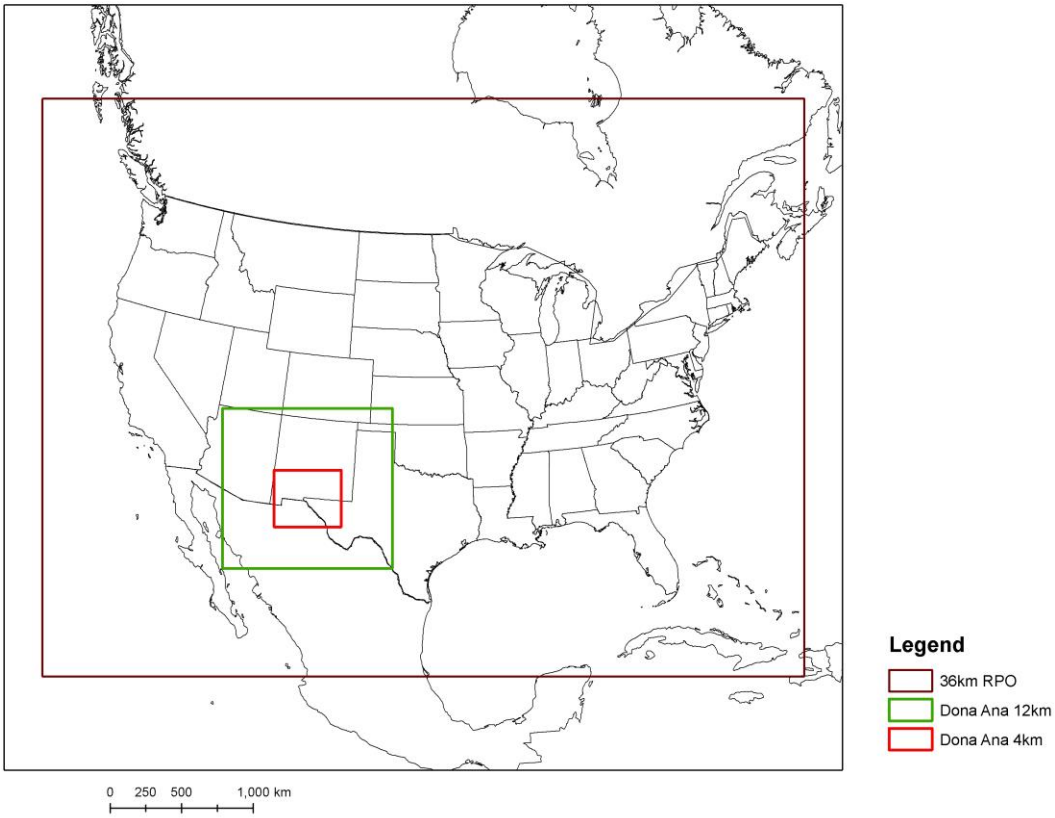

Figure 3. SNMOS 2025 CAMx source apportionment 36/12/4-km modeling domains.

4.2. Vertical Domain Structure

The SNMOS WRF and CAMx modeling will use the vertical domain structure shown in Table 5. WRF will be run with 33 vertical layer interfaces (32 vertical layers using the CAMx definition of layer thicknesses). The WRF model employs a terrain following coordinate system defined by pressure, using multiple layers that extend from the surface to 50 mb (approximately 19 km above mean sea level). No layer averaging (collapsing) scheme will be adopted for the CAMx simulations; CAMx will use the same vertical layers as WRF. The 32 layer structure presented here is unique to the SNMOS and is designed to resolve the impacts of local, regional, and long-range sources of air pollution on receptor sites in the 4-km SNMOS modeling domain. The shallow layers (< 42m) near the surface are configured to resolve the boundary layer dynamics that are crucial to simulating ground-level emissions and air pollution. Maintaining relatively shallow layers (< 2km) aloft without layer collapsing is designed to improve the simulation of stratosphere-troposphere ozone exchange. More layers aloft will also improve the simulation of the impacts of long-range air pollutant transport on regional background air quality.

Table 5. 33 vertical layer interface definition for WRF and CAMx simulations.

WRF and CAMx Levels				
WRF Level	**Sigma**	**Pressure (mb)**	**Height (m)**	**Thickness (m)**
33	0.0000	50.00	19260	2055
32	0.0270	75.65	17205	1850
31	0.0600	107.00	15355	1725
30	0.1000	145.00	13630	1701
29	0.1500	192.50	11930	1389
28	0.2000	240.00	10541	1181
27	0.2500	287.50	9360	1032
26	0.3000	335.00	8328	920
25	0.3500	382.50	7408	832
24	0.4000	430.00	6576	760
23	0.4500	477.50	5816	701
22	0.5000	525.00	5115	652
21	0.5500	572.50	4463	609
20	0.6000	620.00	3854	461
19	0.6400	658.00	3393	440
18	0.6800	696.00	2954	421
17	0.7200	734.00	2533	403
16	0.7600	772.00	2130	388
15	0.8000	810.00	1742	373
14	0.8400	848.00	1369	271
13	0.8700	876.50	1098	177
12	0.8900	895.50	921	174
11	0.9100	914.50	747	171
10	0.9300	933.50	577	84
9	0.9400	943.00	492	84
8	0.9500	952.50	409	83
7	0.9600	962.00	326	83
6	0.9700	971.50	243	81
5	0.9800	981.00	162	65
4	0.9880	988.60	97	41
3	0.9930	993.35	56	32
2	0.9970	997.15	24	24
1	1.0000	1000	0	

5. Modeling Specifications

This chapter describes the modeling software and approaches that will be used for the SNMOS 2011 base and future year simulations. The SNMOS will use the following models for simulating meteorology, emissions, ozone, and other gaseous pollutants in Southern New Mexico.

- Meteorology Model – The non-hydrostatic version of the Advanced Research version of the Weather Research Forecast (WRF-ARW) model version 3.7.1 (Skamarock et al. 2004; 2005; 2006).
- Emissions Processor – Sparse Matrix Operator Kernel Emissions (SMOKE) processor, version 3.7 (UNC, 2015).
- Biogenic Emissions Model – Model of Emissions of Gases and Aerosols from Nature (MEGAN), version 2.10 (Guenther et al., 2012).
- WRAP Windblown Dust Model (WRAP WBD, Mansell et al., 2006).
- Photochemical Grid Models (PGM) – The Comprehensive Air Quality Model with Extensions (CAMx) version 6.20 (ENVIRON, 2015).

5.1. Meteorological Modeling

The WRF meteorological model will be applied for the 2011 calendar year using the 36/12/4-km horizontal domain and 37 layer vertical structures defined above in Chapter 4. WRF will be run from April 15 through September 1, 2011 and the results will be evaluated against surface meteorological observations of wind speed, wind direction, temperature, humidity, and precipitation. The WRF model performance will be compared against meteorological modeling benchmarks and with past regional meteorological model performance evaluations (UNC and ENVIRON, 2012). The WRF precipitation fields will be compared against daily analysis fields from the Parameter-elevation Relationships on Independent Slopes Model (PRISM) for active monsoon periods. The following periods have been identified for detailed analysis as they cover times when the North American Monsoon overlapped with high ozone periods in parenthesis:

- July 25-29 (July 28).
- August 3-5 (August 2-3).
- August 19-22 (August 21).

In advance of the operational WRF simulations that will be used to drive the emissions and PGM modeling, we will conduct a series of sensitivity tests to find the optimal configuration for simulating summer season ozone. In particular, we will focus on simulating the North American Monsoon with an emphasis on the timing, location, and magnitude of precipitation in the region. The sensitivity tests that we propose are based on previous WRF modeling studies of the region and the performance problems that WRF has in simulating convective precipitation in the Western U.S.

- The Bureau of Land Management's Montana-Dakotas (BLM-MT/DK) Study examined the sensitivity of WRF model performance in the Montana/Dakotas region for different WRF model configurations used in recent studies (McAlpine et al., 2014). In the initial Montana-Dakotas modeling, WRF overstated precipitation over the 4-km modeling domain during the summer months. The initial WRF run used surface temperature and humidity observation nudging in the 4-km domain. The temperature and humidity

observation nudging introduced instabilities in the WRF simulation that resulted in increased convective activity and rainfall. BLM-MT/DK Study sensitivity testing demonstrated that removing temperature and humidity observation nudging and using the Grell-Freitas cumulus parameterization on the 4-km domain for the final WRF simulation improved rainfall as well as the wind speed and direction model performance. The reduction in explicit convective activity allowed the WRF to more accurately simulate the observed winds.

- In the San Juan Mercury Modeling (Ramboll Environ and Systech Water Resources, 2015), WRF overpredicted precipitation in a 12-km domain focused on the Four Corners region, but was much more accurate at the 4 km resolution. Observational nudging was applied to the 12-km and 4-km domains for winds, but not for temperature or humidity. Several cumulus parameterizations were evaluated to determine their effect on modeled precipitation.
- The 2011 WRF evaluation for the 3-State Air Quality Study (3SAQS) compared WRF 3.6.1 estimates to monthly PRISM observations (UNC and ENVIRON, 2014). While summertime WRF precipitation was generally too high relative to PRISM and the model did not resolve the local convective features well, there were questions about the PRISM analysis fields and their reliability at capturing isolated convective cells.

In consideration of these WRF studies, we will conduct a series of WRF simulations and select the best performer (lowest bias and error for surface temperature, winds, humidity, and precipitation at sites in the 4-km SNMOS domain) for the operational simulations. The sensitivities will be based off of the WAQS (UNC and ENVIRON, 2014) and San Juan Mercury Modeling (Ramboll Environ and Systech Water Resources, 2015) studies. Table 6 summarizes the base configuration that we will use for the WRF sensitivities and compares this configuration to the WAQS WRF modeling. We will simulate the 36/12/4-km modeling domains for the entire Study period and evaluate the results against surface observations. The evaluation will focus on the shorter time-period North American Monsoon and high ozone episodes identified above. The WRF version 3.7.1 simulations that we will run include the following:

- Configuration 1: Base WRF configuration using settings from the 3SAQS/WAQS 2011 configuration. The key parameters here for the WRF sensitivity tests are the NAM ICBCs and the modified Kain-Fritsch cumulus scheme. The modified convective parameterization scheme provides subgrid-scale cloud fraction and condensate feedback to the shortwave and longwave radiation schemes. The impact of including the subgrid-scale cloud fraction is a reduction in the shortwave radiation, leading to less buoyant energy, thereby alleviating the overly energetic convection and thus a reduction in precipitation.

- Configuration 2: Same as Configuration 1 with the multi-scale (grid-aware) Kain-Fritsch (MSKF) cumulus scheme. Additional changes were made to the modified Kain-Fritsch scheme to improve the accuracy of precipitation at gray zone resolutions (<10km). These include scale dependent features of convection such as scale dependent consumption of the convective available potential energy and entrainment of environmental air.

- Configuration 3: Same as Configuration 2 but using the ECMWF ERA-Interim as the ICBC fields. Experience from the San Juan Hg WRF tests indicate that the ERA-Interim

ICBC fields may improve simulated precipitation associated with the North American Monsoon

- Configuration 4: This WRF sensitivity is optional based on available time and the performance of Configurations 1-3. Configuration 4 is the same as Configuration 3 but based on prior experiences from the San Juan Hg study. Analysis nudging was not applied in domain 2 in the San Juan Hg study. This configuration will turn off analysis nudging for domain 2.

Table 6. Base configuration for the SNMOS WRF sensitivity modeling.

WRF Treatment	3SAQS/WAQS	SNMOS
Microphysics	Thompson	Thompson
Longwave Radiation	RRTMG	RRTMG
Shortwave Radiation	RRTMG	RRTMG
Minutes between radiation physics calls	20	20
Land Surface Model (LSM)	NOAH	NOAH
Planetary Boundary Layer (PBL) scheme	YSU	YSU
Cumulus parameterization	Kain-Fritsch in the 36-km and 12-km domains only.	Kain-Fritsch in the 36-km and 12-km domains only.
Analysis nudging	Applied to winds (uv), temperature (t) and moisture (q) in the 36-km and 12-km domains	Applied to winds (uv), temperature (t) and moisture (q) in the 36-km and 12-km domains
Analysis nudging coefficients	uv: 5e-4 (d01), 3e-4 (d02) t: 5e-4 (d01), 3e-4 (d02) q: 1e-5 (d01 and d02)	uv: 5e-4 (d01), 3e-4 (d02) t: 5e-4 (d01), 3e-4 (d02) q: 1e-5 (d01 and d02)
Observation Nudging	Applied to surface wind and temperature in the 4-km domain	None
Observation nudging coefficients	uv: 1.2e-3 (d03) t: 6e-4 (d03)	N/A
Initialization Dataset	12-km North American Model (NAM)	Decided after analysis of sensitivity modeling experiments
Top (mb)	50	50
Vertical Levels (Layers)	37 (36)	33 (32)

While the final WRF configuration will depend on the results of the sensitivity modeling, details of the WRF input data preparation procedures and model configuration that we will use for the 2011 SNMOS modeling are provided below.

5.1.1. Model Selection

The publicly available version of WRF (version 3.7.1) will be used in the modeling study. We are recommending this latest release version of WRF over the version used for the WAQS (version 3.6.1) to take advantage of the grid-aware MSKF scheme, which may improve the skill of the model at simulating convective precipitation. Additional details of the logic behind the meteorology model selection are provided in Section 2.1.1. The WPS preprocessor programs including GEOGRID, UNGRIB, and METGRID will be used to develop model inputs. A

program developed in-house at UNC-IE for the WAQS project will process SNODAS snow-cover/snow-depth data for input to WRF.

5.1.2. Domain Definitions

The WRF 36/12/4-km domains are defined with at least a 5-grid cell buffer in all directions from the CAMx air quality modeling domains to minimize any potential numeric noise along the WRF domain boundaries, which can affect the air quality model meteorological inputs. Such numeric noise can occur near the boundaries of the WRF domain solution as the boundary conditions come into balance with the WRF numerical algorithms. The WRF modeling will be based on 32 vertical layers with a surface layer approximately 24 meters deep. Details of the domain selection are provided in Chapter 4.

5.1.3. WRF Configuration Specifications

5.1.3.1. Topographic Inputs

Topographic information for the WRF will be developed using the standard WRF terrain databases available from the National Center for Atmospheric Research (NCAR). The 36-km CONUS domain will use the 10 min. (18 km) global data. The 12-km WESTUS domain will use 2 min. (~4 km) data and the 4-km SNMOS domain will be based on the 30 sec. (~900 m) data.

5.1.3.2. Vegetation Type and Land Use Inputs

Vegetation type and land use information will use the most recently released WRF databases provided with the WRF distribution. Standard WRF surface characteristics corresponding to each land use category will be used for this application.

5.1.3.3. Atmospheric Data Inputs

The WRF simulation will either be initialized with the 12-km (Grid #218) North American Model (NAM) archives available from the National Climatic Data Center (NCDC) National Operational Model Archive and Distribution System (NOMADS) server or the 80-km ERA Interim archives from the European Center for Medium-Range Weather Forecasts (ECMWF). The choice of initialization data will be based on the results of the WRF sensitivity modeling described above.

5.1.3.4. Time Integration

Third-order Runge-Kutta integration with a fixed time step of 90 seconds for the 36-km CONUS domain, 30 seconds for 12-km WESTUS domain, and 10 seconds for the 4-km SNMOS domain.

5.1.3.5. Diffusion Options

Horizontal Smagorinsky first-order closure with sixth-order numerical diffusion and suppressed up-gradient diffusion.

5.1.3.6. Lateral Boundary Conditions

Lateral boundary conditions will be specified from the initialization dataset on the 36-km CONUS domain with continuous updates nested from the 36-km domain to the 12-km WESTUS

domain and continuous updates nested from the 12-km domain to the 4-km domain (i.e., one-way nesting with no feedback from the finer to coarser grids).

5.1.3.7. Top and Bottom Boundary Conditions

The top boundary condition will use an implicit Rayleigh dampening for the vertical velocity. Consistent with the model application for non-idealized cases, the bottom boundary condition will be specified as physical, not free-slip.

5.1.3.8. Water Temperature Inputs

NCEP RTG global one-twelfth degree analysis.[2]

5.1.3.9. Snow Cover and Snow Depth

SNODAS observed snow cover and snow depth data will be used to replace the WRF snow forecasts

5.1.3.10. FDDA Data Assimilation

The WRF model will be run with analysis nudging only; observation nudging (i.e., Four Dimensional Data assimilation [FDDA]) will not be used for the SNMOS WRF modeling. The operational nudging configuration is based on the WAQS WRF modeling. Analysis nudging will be used on the 36-km and the 12-km domain. Analysis nudging will not be used on the 4-km domain. Table 6 shows the analysis nudging coefficients that we will use for the operational simulation. Both surface and aloft nudging will be used, though nudging for temperature and mixing ratio will not be performed in the lower atmosphere (i.e., within the boundary layer).

Depending on the results from the first three WRF sensitivities above, we may test a configuration that turns off analysis nudging in the 12-km domain (only using nudging in the outer 36-km domain). This simulation will only be performed if we do not obtain acceptable model performance from one of the first three WRF sensitivity configurations.

5.1.3.11. Physics Options

The possible base WRF physics options chosen for this application are presented in Table 6. The best-performing physics options configurations will be selected after performing the WRF sensitivity tests described above. Several physics options will not change across the different sensitivity simulations and are based on a review of several years worth of WRF modeling across the Western U.S.:

- Thompson ice, snow, and graupel scheme (mp_physics=8)
- RRTMG long wave radiation (ra_lw_physics=4)
- RRTMG short wave radiation (rw_sw_physics=4)
- Monin-Obukhov surface layer (sf_sfclay_physics=1)
- Unified NOAH land-surface model (sf_surface_physics=2)
- YSU planetary boundary layer scheme (bl_pbl_physics=1)

[2] Real-time, global, sea surface temperature (RTG-SST) analysis. http://polar.ncep.noaa.gov/sst/oper/Welcome.html.

The cumulus parameterization is the physics option that will change based on the results of the WRF sensitivity tests. In particular, the choice of whether to use the new grid-aware Kain-Fritsch (MSKF) scheme will be resolved through the sensitivity modeling.

5.1.4. Application Methodology

The WRF model will be executed in 5-day blocks initialized at 12Z every 5 days with a 90-second integration time step. Model results will be output every 60 minutes and output files split at 24-hour intervals. Twelve hours of spin-up will be included in each 5-day block before the data are used in the subsequent evaluation. The model will be run at the 36-km, 12-km and 4-km grid resolution from May 15 through September 1, 2011 using one-way grid nesting with no feedback (i.e., the meteorological conditions are allowed to propagate from the coarser grid to the finer grid but not vice versa).

5.1.5. Evaluation Approach

The model evaluation approach will be based on a combination of qualitative and quantitative analyses. The quantitative analysis are divided into monthly summaries of 2-m temperature, 2-m mixing ratio, and 10-m wind speed using the boreal seasons to help generalize the model bias and error relative to a standard benchmark. The evaluation will focus on the 4-km domain and sites within New Mexico. The evaluation will be supplemented with select diurnal and time series analyses at specific sites. Additional analysis will include a qualitative evaluation of the daily total WRF precipitation fields against PRISM fields. The PRIMS data will be mapped to the WRF domains and grid resolution. The observed database for winds, temperature, and water mixing ratio to be used in this analysis are the National Oceanic and Atmospheric Administration (NOAA) Earth System Research Laboratory (ESRL) Meteorological Assimilation Data Ingest System (MADIS).

5.2. Emission Modeling

The section presents the emissions database that we will use for the SNMOS modeling.

Emissions data fall into three broad categories:

- Inventory data – county total estimates of emissions from explicit source categories that have 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 that are 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 that are typically used with SMOKE or another emission model to generate the hourly gridded PGM-ready emissions inputs.

The SNMOS modeling will use the base and future year WAQS 2011b emissions data and configurations. Details of the SNMOS emissions simulations are provided below.

5.2.1.1. 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 are inventoried with 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 as either mobile or non-mobile sources, with special characteristics required for mobile sources. Descriptions of the different inventory sectors used for the SNMOS modeling, including the sources of these data, are provided in this section.

Consistent with the WAQS 2011b emissions modeling platform, all of the non-O&G anthropogenic emission inventories for the SNMOS base year 2011 and future year 2025 simulations will be taken from the U.S. EPA National Emission Inventory (NEI). EPA publically released the 2011v6 platform in February 2014 and updated it twice, version 6.2 being the most recent. Details of the inventory, sectors, and preparation procedures for these data are available in the NEI2011v6.2 Technical Support Document (EPA, 2015).

We will use the same emissions processing sectors as were used for the WAQS Base11b modeling. These sectors differ slightly from the NEI2011v6 platform and were developed to facilitate reporting, quality assurance, and special processing of the data. **Error! Reference source not found.**Table 7 lists the emission inventory sectors that were used for the WAQS 2011b modeling and will also be used for this Study.

Table 7. SNMOS emissions inventory sectors

Sector	Source	Type	Inventory Period and Year	Description
Locomotive/ marine	NEI 2011v6.2	Point and Nonpoint	Annual 2011 and 2025	The locomotive/marine sector is a subset of the non-point/area sector. It includes county-level emissions for line haul locomotives (nonpoint), train yards (point), and class 1 and 2 in- and near-shore commercial marine
Off-road mobile	NEI 2011v6.2	Nonpoint	Monthly 2011 and 2025	NMIM 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. The CA and TX NONROAD estimates were normalized to emissions values provided by these states.
On-road mobile (US)	NEI 2011v6.2	MOVES	Annual and Daily 2011 and 2025	EPA ran MOVES2014 for 2011 in emissions factor mode. The MOVES lookup tables include on-network (RPD), on-network refueling (RPD_RFL), on-network for CA and TX (RPD_CATX), off-network starts/stops (RPV), off-network starts/stops refueling (RPV_RFL), off-network starts/stops for CA and TX (RPV_CATX), off-network vapor venting (RPP), off-network vapor venting sources for CA and TX (RPP_CATX), off-network hotelling (RPH). These data include the reference county and reference fuel month assignments that EPA used for the MOVES simulations. The CA and TX MOVES estimates were normalized to emissions values provided by these states.

Sector	Source	Type	Inventory Period and Year	Description
Non-point/ Area	NEI 2011v6.2	Nonpoint	Annual 2011 and 2025	County-level emissions for sources that individually are too small in magnitude or too numerous to inventory as individual point sources. Includes small industrial, residential, and commercial sources; broken out into nonpoint, residential wood combustion, livestock, and fertilizer processor sectors
Area Oil & Gas	WAQS 2011 and NEI 2011v6.2	Nonpoint	Annual 2011 and 2020	Non-point oil and gas sources are survey-based and typically unpermitted sources of emissions from up-stream oil and gas exploration, development, and operations. The non-point O&G sector consists of the WAQS Phase II and the NEI 2011v6.2 inventory for all basins outside of the WAQS inventory coverage area.
Point Oil & Gas	WAQS 2011 and NEI 2011v6.2	Point	Annual 2011 and 2020	Point oil and gas sources are permitted sources of emission from up-stream oil and gas exploration, development, and operations. The point O&G sector consists of the WAQS Phase II and the NEI 2011v6.2 inventory for all areas outside of the WAQS inventory coverage area
CEM Point	2011v6.2 and CAMD	Point	Hourly 2011 and 2025	2011 Clean Air Markets Division (CAMD) hourly Continuous Emissions Monitor (CEM) data and Integrated Planning Model (IPM) projections to 2025
non-CEM Point	2011v6.2	Point	Annual 2011 and 2025	Elevated and low-level combustion and industrial sources, airports, and offshore drilling platforms.
Offshore Shipping	2011v6.2	Point	Annual 2011 and 2025	Elevated point C3 commercial marine sources in offshore commercial shipping lanes
Fires	PMDETAIL	Point	Daily 2011	PMDETAIL version 2
Canada Sources	NPRI 2010	Nonpoint and Point	Annual 2010	Canadian 2010 National Pollutant Release Inventory; there are no future year projections from the 2010 NPRI
Mexico Sources	MNEI 2012	Nonpoint and Point	Annual 2008 and 2025	Mexican NEI 2008 and projections to 2025
Biogenic	MEGAN v2.10	Gridded	Hourly 2011	MEGANv2.10 estimated with 2011 meteorology
Windblown Dust	WRAP WBD	Gridded	Hourly 2011	WRAP Windblown Dust Model (WBD) estimated with 2011 meteorology
Sea Salt	Ramboll Environ	Gridded	Hourly 2011	Sea salt emissions estimated with 2011 meteorology
Lightning	Ramboll Environ	Gridded	Daily 2011	Lightning NOx emissions estimated with 2011 meteorology

5.2.1.2. Gridded Data

Several gridded datasets will be used for either directly estimating air emissions or as ancillary data for processing/adjusting the emissions data. The following datasets are key gridded data that will be used for the SNMOS. Note that all of the gridded emissions data listed here will be held constant at the year 2011 levels in the 2025 future modeling. The reasons for holding these emissions constant in the future simulations is because land use projections and for fires, fuel loading and activity forecasts, are both difficult to obtain and highly uncertain.

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)

The gridded data for input to the MEGANv2.10 biogenic model that will be used to estimate 2011 biogenic emissions for the SNMOS include the following:

- Leaf Area Index (LAI): A gridded dataset of 46 8-day files for North America were generated for 2011 at 1-km resolution
- Plant Functional Type (PFT): A gridded dataset of 9 PFTs were developed at both 1-km and 56-m resolutions across the modeling domains.
- Photsynthetically Active Radiation (PAR): Satellite PAR gap-filled with WRF solar radiation fields scaled by a factor of 0.45
- Additional details on the development and evaluation of the gridded data to be used for this Study are available in the final report on the WRAP Biogenic Emissions Study (Sakulyanontvittaya, Yarwood and Guenther, 2012).
- SNMOS 2011 WRF meteorology

Fire Emissions

Open biomass burning makes up an important part of the total global emissions of greenhouse gases, reactive trace gases, and particulate matter. Although episodic in nature and highly variable, open biomass burning emissions can contribute to local, regional, and global air quality problems and climate forcings. The SNMOS will use fire emissions for 2011 that were generated by the Particulate Matter Deterministic and Empirical Tagging and Assessment of Impacts on Levels (PMDETAIL) study. PMDETAIL developed 2011 fire emission using satellite data and ground detect and burn scar, in addition to other data, with a slight modification (Mavko, 2014) to the methodology used in the Deterministic and Empirical Assessment of Smoke's Contribution to Ozone Project (DEASCO3) study for the 2008 modeling year (DEASCO3, 2013). We will use a similar plume rise approach as PMDETAIL/DEASCO3 where plume rise depends on fire size and type (Mavko and Morris, 2013). The PMDETAIL 2011 fire inventory was selected over the 2011 Fire INventory from NCAR (FINN) and Smartfire 2011 inventory because it uses a more complete satellite and surface fire dataset.

Windblown Dust (WBD) Emissions

The major components of the WRAP WBD model include:

- Land use/land cover (LULC)
- Soil characteristics
- Surface roughness lengths
- Meteorology (wind-speeds and friction velocities)

The gridded data for input to the WRAP WBD Model that will be used to estimate 2011 emissions for the WAQS include the following:

- Land use/Land cover (LULC): Gridded dataset of 1-km year 2000 North American Land Cover (NALC) regridded to the WestJumpAQMS modeling domains
- Soil characteristics: Gridded 12-category State Soil Geographic Database (STATSGO) mapped to the 4-category classification used in the WRAP WBD
- Surface roughness lengths: Values reported in the literature as of 2006 were mapped to the land use categories in the NALC
- WAQS 2011 WRF meteorology
- Additional details on the development and evaluation of the gridded data to be used for the WAQS are available in the final report on the WRAP WBD (Mansell et al., 2006).

Sea Salt

R-E 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 that will be used for the WAQS is a land-water mask file that identifies each modeling domain grid cell as open ocean, surf zone, or land. Additional details on the development and evaluation of the sea salt emissions processor to be used for the SNMOS are available in the WestJumpAQMS Sea Salt and Lightning memo (Morris, Emery, Johnson and Adelman, 2012).

The SNMOS will use the CAMx sea salt emissions processor with 2011 WRF data to generate sea salt emissions for the 36 and 12-km modeling domains. The SNMOS 4-km domain is inland and will not have any sea salt emissions.

Lightning

The modified lightning NOx emissions model of Koo et al. (2010) used in the WAQS will be used to estimate lightning NOx emissions for the SNMOS. Additional details on the development and evaluation of the lightning emissions processor used for the WAQS are available in the WestJumpAQMS Sea Salt and Lightning memo (Morris, Emery, Johnson and Adelman, 2012).

Fugitive Dust Transport Factors

Transport factors are applied to the primary dust emissions estimates to adjust the emissions for vegetative scavenging. The dust models and emissions factors are based on soil characteristics and do not account for the presence of vegetation, which has a mitigating effect on both winds and dust emissions. An ad-hoc approach of adjusting dust emissions estimates has been developed that uses gridded land cover data to simulate the impacts of vegetation cover on dust.

For the SNMOS 2011 modeling we will use dust transport factors collected for the WAQS, which were derived from 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 the transport factors gridded to each of the SNMOS modeling domains to reduce the dust emissions.

5.2.1.3. Ancillary Emissions Data

Ancillary emissions data includes all of 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. Data files called spatial surrogates are used to map the county-level emission inventories to the model grid cells. Spatial surrogates are generated from Geographic Information System (GIS) Shapefiles using software that calculates the fractions of county-level different geospatial attributes in a model grid cell.

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. With the exception of a few source types (e.g. Continuous Emissions Monitoring data, biogenic emissions, windblown dust and some fire inventories), most inventory data include annual or daily emission estimates. Temporal profiles are used to compute hourly emissions from the annual or daily inventory estimates. The SMOKE model, which is being used to process emission for the SNMOS, uses three types of temporal profiles:

- Monthly profiles: Convert annual inventory to monthly emissions accounting for seasonal and other effects.
- Daily profiles: Convert monthly emissions to daily emissions accounting for day-of-week and other effects.
- 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. The emissions inventories for the SNMOS include 6 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 diameter < 2.5 micrometers ($PM_{2.5}$). Chemical speciation profiles are used to describe the chemical compositions of the effluent from particular emissions sources. The exact specification of the source-specific emissions species is determined by the chemistry mechanism selected for the AQM simulation. Speciation profiles convert the inventory pollutants to more detailed source-specific species in terms required by the AQM chemistry mechanism.

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).

The ancillary data for SNMOS will be taken directly from the WAQS 2011b modeling, which was derived primarily from the EPA 2011v6.2 modeling platform.

5.2.1.4. Emissions Processing

SMOKE version 3.7 (September 2015 release) will be used to process all of the emissions sectors other than fires, biogenics, windblown dust, sea salt, and lightning. The procedures for processing emissions for generating CAMx emission inputs using SMOKE are described below. The name of the SMOKE progam used for each step is listed in parentheses.

- Import (Smkinven) – read raw inventory files

  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

- Grid (Grdmat) – read and match spatial surrogates to inventory sources and assign the emissions to PGM grid cells

  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

- Speciation (Spcmat) – read and match VOC and PM chemical profiles to inventory sources and calculate emissions in terms of PGM species

  Convert inventory VOC to total organic gases (TOG) for consistency with the NEI SPECIATE speciation profiles, where POLLUTANT_CONVERSION = Y

- Temporal (Temporal) – read and match monthly/week/hourly temporal profiles to inventory sources and estimate hourly emissions

  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 timezone, 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 SNMOS are considered elevated if the effective stack height is greater than 20m

- Create PGM-ready emissions by sector (Smkmerge) – combine all of the intermediate steps above to create a low-level emissions file for each inventory sector and an elevated file for the elevated point sectors

  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 (MOVESMrg) – input mobile activity data and MOVES emission factor look up tables to generated gridded, speciated, hourly emissions

  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

- Final merge (Mrggrid) - Merge the low-level sector emissions to a single file per day

  Create CAMx-ready binary files (Smk2emis) – convert netCDF SMOKE outputs to UAM-formatted data for CAMx

- Merge elevated source (Mrgelev) – combine elevated files to a single file per day and convert to UAM-formatted data for CAMx

While there are four main types of inventory data (point, nonpoint, mobile, and biogenic), as described above, it is necessary to refine 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 the SNMOS 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)

Table 8 defines the emissions categories that we will define for the SNMOS project. The "Temporal" column in this table refers to the temporal configuration that will be used for each category.

Table 8. SNMOS emissions processing sectors

Emissions Processing Category (Abbr)	Temporal	Processing Comments
Nonpoint/Area (nonpt)	mwdss_mon	Remove oil & gas, agricultural NH3, and dust, and includes commercial marine and rail
Livestock NH3 (lv)	mwdss_mon	Met-based temporal profiles;
Fertilizer NH3 (ft)	mwdss_mon	
Fugitive and Road Dust (fd)	mwdss_mon	Includes paved and unpaved road dust; apply transport factors but not met factors
Residential Wood Combustion (rwc)	mwdss_mon	Met-based temporal profiles
Area Oil & Gas (arog)	aveday_mon	Oil and gas sources for the 3SAQS basins; basin specific speciation profiles and spatial surrogates
US Area Oil & Gas (usarog)	aveday_mon	Oil and gas sources outside of the 3SAQS basins
Nonroad mobile (nr)	mwdss_mon	NMIM commercial marine and rail moved to alm
Locomotive/Marine (loma)	mwdss_mon	Includes monthly and annual inventories
MOVES RPD (rpd)	hourly met	Daily emissions factor lookup tables
MOVES RPD Refueling (rpd_rfl)	hourly_met	Daily emissions factor lookup tables
MOVES RPD for CA and TX (RPD_CATX)	hourly_met	MOVES temporal and spatial distribution with magnitudes from CARB and TCEQ
MOVES RPP (rpp)	hourly met	Daily emissions factor lookup tables
MOVES RPP for CA and TX (RPP_CATX)	hourly_met	MOVES temporal and spatial distribution with magnitudes from CARB and TCEQ
MOVES RPV (rpv)	hourly met	Daily emissions factor lookup tables
MOVES RPV Refueling (rpv_rfl)	hourly_met	Daily emissions factor lookup tables
MOVES RPV for CA and TX (RPV_CATX)	hourly_met	MOVES temporal and spatial distribution with magnitudes from CARB and TCEQ
CEM Point (ptcem)	daily	Anomalies removed from 2011 CAMD data
Non-CEM Point (ptncem)	mwdss_mon	Removed oil & gas sources and transferred to ptog sector; includes point aircraft and ports
Point Oil & Gas (ptog)	mwdss_mon	Point oil and gas sources for the WAQS basins
US Point Oil & Gas (usptog)	aveday_mon	Oil and gas sources outside of the WAQS basins
Point Fires (ptfire)	daily	Pre-computed plume rise, processing

Emissions Processing Category (Abbr)	Temporal	Processing Comments
		outside of SMOKE. Separately process for WF, Rx and AGfires.
Commercial Marine (ptseca)	aveday_mon	
Canada Area (canar)	mwdss_mon	Canadian National Pollutant Release Inventory for 2010; no future year
Mexico Area (mexar)	mwdss_mon	Mexico National Inventory for 2008; 2025 future year projection
Canada/Mexico Point (nuspt)	mwdss_mon	Canadian National Pollutant Release Inventory for 2010; Mexico National Inventory for 2008; 2025 future year projection for Mexico only
Canada Mobile (canmb)	mwdss_mon	Canadian National Pollutant Release Inventory for 2010; no future year
Mexico Mobile (mexmb)	mwdss_mon	Mexico National Inventory for 2008; 2025 future year projection
Lightning NOx (lnox)	hourly met	Gridded monthly NLCD lightning flash counts converted to hourly, gridded NO emissions with WRF convective rainfall
Sea salt (ss)	hourly met	Surfzone and open ocean PM emissions
Windblown Dust (wbd)	hourly met	
MEGAN Biogenic (bg)	hourly met	Use new versions of MEGAN V2.10 updated by WRAP for the western U.S.

The emissions will be processed by major source category in several different "streams" of emissions modeling. This is done in order 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 with all pre-merged emissions inputs merged together to generate the final CAMx-ready two-dimensional gridded low-level (layer 1) and point source emission inputs.

Quality assurance (QC) of the emissions processing will consist of comparisons of the SNMOS emissions to the WAQS emissions, scrutiny of processing logs, and expert judgment to confirm the quality of the final emissions. We will generate tabulated and graphical summaries of the emissions for comparison with the WAQS 2011b simulation. As each SMOKE program outputs a log file with each cycle, we will use manual and automated procedures to inspect the logs for errors or warnings that may indicate problems with the SMOKE processing or the input data.

5.3. Photochemical Modeling

The SNMOS project will conduct photochemical modeling of the 2011 New Mexico ozone season (May 1 – September 30) on the 36/12/4-km modeling domains shown in Figure 2 using the CAMx photochemical grid model (PGM). The CAMx configuration used for the 2011 base year modeling and the 2025 future year modeling will be directly derived from the WAQS 2011b modeling platform.

Table 9 summarizes the CAMx version 6.20 (March 2015 release) science configuration and options to be used for the 2011 ozone season simulation. CAMx version 6.20 will be configured to predict ozone and PM species as well as nitrogen and sulfur deposition.

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 CB6r2 gas-phase chemical mechanism is selected for CAMx because it includes the very latest chemical kinetic rates and represents improvements over the other alternative CB05 and SAPRC chemical mechanisms as well as active methane chemistry. Additional CAMx inputs will include:

Meteorological Inputs: The WRF-derived meteorological fields will be processed to generate CAMx meteorological inputs using the WRFCAMx processor.

Initial/Boundary Conditions: The boundary conditions (BCs) for the WAQS 36-km CONUS domain simulation to be used in the SNMOS were extracted from a MOZART global chemistry model (GCM) simulation of 2011. MOZART output species were interpolated from the MOZART horizontal and vertical coordinate system to the CAMx LCP coordinate system and vertical layer structure and the MOZART chemical species were mapped to the chemical mechanism used by CAMx. The MOZART dust and sea salt species were zeroed out based on findings from the WAQS 2011 modeling. The WAQS 2011 36-km CONUS CAMx simulation was then driven with the MOZART-derived BCs. The WAQS 2011 12-km modeling was in turn driven with the WAQS CONUS 36-km CAMx outputs as BCs.

The SNMOS 2011 base case modeling will use both 36-km and 12-km WAQS CAMx model output as BCs for the SNMOS WESTUS12 grid shown in Figure 2. The WESTUS12 CAMx modeling domain has been extended southward beyond the southern boundary of the WAQS 12-km modeling domain in order to include the Carbon II coal-fired power plant. This facility is a large source of NOx emissions and lies in a region that was sometimes upwind of Doña County on high ozone days during 2011.

For the SNMOS 2011 modeling, we will extract BCs for the WESTUS12 domain northern boundary from the WAQS 12-km modeling. We will also use BCs extracted from the WAQS 12-km domain for the portions of the eastern and western WESTUS12 boundary that lie within the WAQS 12-km domain. For the WESTUS12 domain southern boundary and the portions of the eastern and western boundary that lie outside the WAQS 12-km domain, we will extract BCs from the WAQS 36-km CONUS simulation. The CAMx BNDEXTR_v6 tool will be adapted to carry out this procedure.

For the 2025 future year source apportionment modeling, we will use a nested 36/12/4-km model configuration to allow detailed source apportionment identifying contributions from regions outside the 12 km grid, but within the 36 km grid.

Photolysis Rates: The modeling team will prepare the photolysis rate inputs as well as albedo/haze/ozone/snow inputs for CAMx. Day-specific ozone column data will based on the Total Ozone Mapping Spectrometer (TOMS) data measured using the satellite-based Ozone Monitoring Instrument (OMI). Albedo will be based on land use data. For CAMx there is an ancillary snow cover input that will override the land use based albedo input. Average values for typical snow cover will be utilized. Although we are simulating a late spring/summer episode, there are mountains exceeding 3,000 m above ground level within the 12-km domain where snow may be present during the modeling period. For CAMx, the TUV photolysis rate processor will be used. If there are periods of more than a couple of days where daily TOMS data are unavailable, the TOM measurements will be interpolated between the days with valid data; in the

case large periods of TOMS data are missing monthly average TOMS data will be used. CAMx will also be configured to use the in-line TUV to adjust for cloud cover and account for the effects aerosol loadings have on photolysis rates; this latter effect on photolysis may be especially important in adjusting the photolysis rates due to the occurrence of PM concentrations associated with emissions from fires.

Landuse: We will generate landuse fields based on USGS GIRAS data.

Spin-Up Initialization: A minimum of ten days of model spin up will be performed on the 2011 CAMx 12/4 km grid before the first day with MDA8 ozone>70 ppb at any Dona Ana County ozone monitor. For the 2025 modeling, there will be a 14 day spinup on the nested 36/12/4 km grids before the first simulation day.

Table 9. SNMOS CAMx version 6.20 configuration

Science Options	Configuration	Details
Model Codes	CAMx V6.20 – March 2015 Release	
Horizontal Grid Mesh	36/12/4 km	
36 km grid	148 x 112 cells	36-km CONUS domain
12 km grid	99 x 93 cells	12-km SNMOS WESTUS12 regional domain
4 km grid	117 x 99 cells	4-km Dona Ana domain
Vertical Grid Mesh	34 vertical layers defined by WRF; no layer collapsing	Layer 1 thickness ~12 m. Model top at ~19-km above MSL
Grid Interaction	12/4-km two-way nesting for CAMx (2011) 36/12/4-km two way nesting for CAMx (2025)	
Initial Conditions	10 day spin-up on 12/4 km grid before first day with MDA8 ozone>70 ppb at any Dona Ana County monitor (2011) 14 day spin-up on 36/12/4 km grid (2025)	Clean initial conditions
Boundary Conditions	12 km SNMOS grid from 36/12-km WAQS modeling (2011) 36 km grid from global chemistry model (2025)	MOZART GCM data for 2011; zero out dust and sea salt.
Emissions		
Baseline Emissions Processing	SMOKE, MOVES and MEGAN	
Sub-grid-scale Plumes		
Chemistry		
Gas Phase Chemistry	CB6r2	Active methane chemistry and ECH4 tracer species
Meteorological Processor	WRFCAMx	Compatible with CAMx V6.20
Horizontal Diffusion	Spatially varying	K-theory with Kh grid size dependence
Vertical Diffusion	CMAQ-like in WRF2CAMx	
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 2003
Wet Deposition	CAMx-specific formulation	rain/snow/graupel/virga

Science Options	Configuration	Details
Numerics		
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	Collela and Woodward (1984)
Integration Time Step	Wind speed dependent	~0.1-1 min (4 km), 1-5 min (1 -km), 5-15 min (36 km)

6. CAMx Model Performance Evaluation

Using the inputs and model configurations described here, an initial CAMx 2011 base case simulation will be conducted for the 12 and 4-km modeling domains and the 2011 ozone season. The SNMOS_2011a CAMx simulation results for O_3, carbon monoxide (CO), nitrogen dioxide (NO_2), 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 EPA's photochemical modeling guidance documents (EPA, 2014d) and described in detail in the WAQS 2011 Model Performance Evaluation Final Report (Adelman, Shanker, Yang and Morris, 2015). While the focus of the SNMOS is on O_3, a cursory evaluation of the PM performance will be conducted to assess the overall validity of the model for the application period and domains.

Detailed evaluation of O_3 and precursor species will focus on the model performance at monitors in the 4-km modeling domain. **Error! Reference source not found.** is a map of the SNMOS modeling region showing the locations of air quality monitors that will be used for the CAMx evaluation. This map highlights that there is a cluster of AQS and CSN monitors in the Doña Ana County region extending from Las Cruces southeast to El Paso and Ciudad Juarez. The data from these monitors will be key inputs to the evaluation of the surface O_3 and PM concentrations predicted by CAMx.

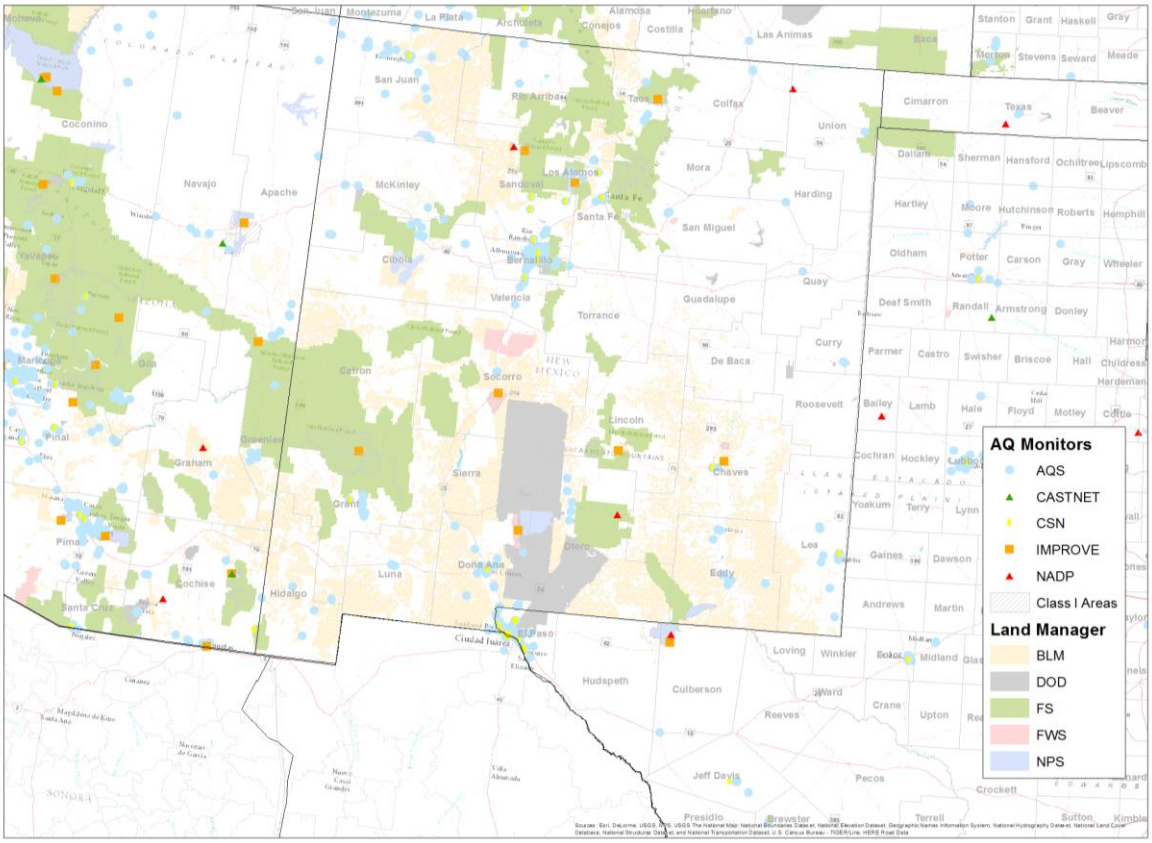

Figure 4. Air quality monitors in New Mexico and the surrounding area

6.1. Available Aerometric Data for the model Evaluation

The following routine air quality measurement data networks operating in in 2011 will be used in the SNMOS model performance evaluation:

EPA AQS Surface Air Quality Data: Data files containing hourly-averaged concentration measurements at a wide variety of state and 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. The standard hourly AQS AIRS monitoring stations typically measure hourly ozone, NO_2, NO_X and CO concentration and there are thousands of sites across the U.S. The Federal Reference Method (FRM) network 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 time period using a 1:3 or 1:6 day sampling frequency.

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 a large number of sites located in the western U.S. Although there are also some IMPROVE protocol sites that can be more urban-oriented.

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 collected hourly ozone, 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).

NADP Network: The National Acid Deposition Program (NADP) collects weekly samples of SO_4, NO_3 and NH_4 in precipitation (wet deposition) in their National Trends Network (NTN) at over a 100 sites across the U.S. that are mainly located in rural areas away from big cities and major point sources. Seven NADP sites also collect daily wet deposition measurements (AIRMON) when precipitation occurs. Over 20 of the NADP sites also collect weekly mercury (MDN) samples. Figure 4 shows the locations of the NADP NTN, AIRMoN and MDN monitoring sites. Note that observed sulfate and nitrate dry deposition can be estimated at CASTNet sites using concentrations and a micro-meteorological model that produces a deposition velocity. But these are not true observations, but model estimates of the observations.

6.2. Model Performance Statistics, Goals and Criteria

For over two decades, ozone model performance has been compared against EPA's 1991 ozone modeling guidance performance goals (EPA, 1991). For PM species a separate set of model performance statistics and performance goals and criteria have been developed as part of the regional haze modeling performed by several Regional Planning Organizations (RPOs). EPA's modeling guidance notes that PM models might not be able to achieve the same level of model performance as ozone 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, several researchers have developed PM model performance goals and criteria that are less stringent than the ozone goals as shown in Table 10 (Boylan, 2004; Boylan and Russell, 2006; Morris et al., 2009a,b).

Table 10. Ozone and PM model performance goals and criteria

Fractional Bias (FB)	Fractional Error (FE)	Comment
≤±15%	≤35%	Ozone model performance goal that would be considered very good model performance for PM species
≤±30%	≤50%	PM model performance Goal, considered good PM performance
≤±15%	≤35%	PM model performance Criteria, considered average PM performance. Exceeding this level of performance for PM species with significant mass may be cause for concern.

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, Baker and Phillips, 2012). Although these recommendations are not official EPA guidance, they are useful and will be used in the SNMOS model performance evaluation:

- PGM MPE studies should at a minimum report the Mean Bias (MB) and Error (ME or RMSE), and 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 ozone using an appropriate observed ozone cut-off concentration (3SAQS will use 60 ppb).
- The model evaluation statistics should be calculated for the highest resolution temporal resolution available and for important regulatory averaging times (e.g., daily maximum 8-hour ozone).
- 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., SO4, NO3, NH4, EC, OA and OPM2.5).
- Evaluation should be performed for subsets of the data including, high observed concentrations (e.g., ozone > 60 ppb), by subregions and by season or month.
- Evaluation should include more than just ozone 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 in order to make meaningful interpretation of the model performance evaluation.

We will incorporate the recommendations of Simon, Baker and Philips (2012) into the SNMOS model performance evaluation as data are available. The SNMOS 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) ozone, including MDA8 with a 60 ppb threshold
- Carbon monoxide, nitrogen dioxide, NO_2, volatile organic compounds (VOCs, if available)
- Total $PM_{2.5}$, elemental carbon, organic carbon, sulfate, nitrate, ammonium, and visibility metrics
- Vertical ozone comparisons to ozonesonde and available aircraft observation data

6.2.1.1. Model Evaluation Tools

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

- PAVE and VERDI: The Package for Analysis and Visualization (PAVE) and Visualization Environment for Rich Data Interpretation (VERDI) are visualization tools specifically designed to visualize photochemical grid model output. They can run on both a Linux and Windows environment, so can be used while the photochemical grid model

is running or has recently been completed. Both tools are primarily used for spatial maps where modeled tile plots can be displayed with superimposed observations. VERDI can also generate scatter and time series plots. Although VERDI has replaced PAVE, which is no longer supported, because the modeling community has scripts already set up for PAVE, PAVE is easier to use and VERDI does not have some of the functionality of PAVE, PAVE is still a useful and viable model evaluation tool.

- Excel: The Microsoft Excel spreadsheet software tool is used extensively to generate various model performance displays (e.g., scatter, time series and soccer plots) under Windows. The modeling results and observations must be processed to get them into Excel. But once the data are in Excel, the user has lots of control over the displays.
- AMET: The Atmospheric Model Evaluation Tool (AMET; UNC, 2008) was developed by EPA and consists of MySQL and r code with various scripts for generating the usual model evaluation graphics. It is more difficult to set up than the UCR, PAVE and VERDI tools but can generate useful model evaluation graphics and statistics. AMET will be used extensively for the WAQS 2014pre model performance evaluation.

These tools will be used to develop model performance statistics and graphics similar to those used in the 3SAQS 2011 Model Performance Evaluation Final Report (Adelman, Shanker, Yang and Morris, 2014; 2015).

7. Acronyms

3SAQS	Three-State Air Quality Study
AMET	Atmospheric Model Evaluation Tool
APCA	Anthropogenic Precursor Culpability Assessment
AQ	Air Quality
AQS	Air Quality System
BC	Boundary Condition
BEIS	Biogenic Emissions Information System
BLM	Bureau of Land Management
CAMD	Clean Air Markets Division
CAMx	Comprehensive Air-quality Model with extensions
CARB	California Air Resources Board
CASTNet	Clean Air Status and Trends Network
CB05	Carbon Bond mechanism version 5
CB6r2	Carbon Bond mechanism version 6, revision 2
CEM	Continuous Emissions Monitor
CMAQ	Community Multiscale Air Quality modeling system
CMU	Carnegie Mellon University
CONUS	Continental United States
CPC	Center for Prediction of Climate
CSAPR	Cross State Air Pollution Rule
CSN	Chemical Speciation Network
DEASCO3	Deterministic and Empirical Assessment of Smoke's Contribution to Ozone
DMA	Denver Metropolitan Area
DSAD	Detailed Source Apportionment Domain
ECA	Emissions Control Area
EGU	Electrical Generating Units
EIS	Environmental Impact Statement
EM	Emissions Model
EMS	Emissions Modeling System
EPA	Environmental Protection Agency
EPS	Emissions Processing System
ESRL	Earth Systems Research Laboratory
FB	Fractional Bias
FE	Fractional Error
FLM	Federal Land Manager
FRM	Federal Reference Method
GCM	Global Chemistry Model
GEOS-Chem	Goddard Earth Observing System (GEOS) global chemistry model
IAD	Impact Assessment Domain
IMPROVE	Interagency Monitoring of Protected Visual Environments
IPAMS	Independent Petroleum Association of the Mountain States
IPM	Integrated Planning Model
IWDW	Intermountain West Data Warehouse
LCP	Lambert Conformal Projection
LSM	Land Surface Model
MADIS	Meteorological Assimilation Data Ingest System
MATS	Mercury and Air Toxics Standards
MATS	Modeled Attainment Test Software

MCIP	Meteorology-Chemistry Interface Processor
MEGAN	Model of Emissions of Gases and Aerosols in Nature
MM	Meteorological Model
MM5	Version 5 of the Mesoscale Model
MNGE	Mean Normalized Gross Error
MNB	Mean Normalized Bias
MOVES	Motor Vehicle Emissions Simulator
MOZART	Model for OZone And Related chemical Tracers
NAAQS	National Ambient Air Quality Standard
NADP	National Acid Deposition Program
NCAR	National Center for Atmospheric Research
NCDC	National Climatic Data Center
NEI	National Emissions Inventory
NEPA	National Environmental Policy Act
NMB	Normalized Mean Bias
NME	Normalized Mean Error
NMIM	National Mobile Inventory Model
NOAA	National Oceanic and Atmospheric Administration
NPRI	National Pollutant Release Inventory
OA	Organic Aerosol
OSAT	Ozone Source Apportionment Technology
PA	Process Analysis
PAVE	Package for Analysis and Visualization
PBL	Planetary Boundary Layer
PGM	Photochemical Grid Model
PM	Particulate Matter
PMDETAIL	Particulate Matter Deterministic and Empirical Tagging and Assessment of Impacts on Levels
PPM	Piecewise Parabolic Method
PSAT	Particulate Source Apportionment Technology
QA	Quality Assurance
QC	Quality Control
RMP	Resource Management Plan
SCC	Source Classification Code
SIP	State Implementation Plan
SMOKE	Sparse Matrix Kernel Emissions modeling system
SOA	Secondary Organic Aerosol
TCEQ	Texas Commission on Environmental Quality
UNC	University of North Carolina
UPA	Unpaired Peak Accuracy
USFS	United States Forest Service
VERDI	Visualization Environment for Rich Data Interpretation
VMT	Vehicle Miles Traveled
WBD	Wind Blown Dust model
WAQS	Western Air Quality Study
WESTAR	Western States Air Resources Council
WESTUS	Western United States
WRAP	Western Regional Air Partnership
WGA	Western Governors' Association
WRF	Weather Research Forecasting model

8. References

Adelman, Zachariah. Technical Memorandum: "3SAQS Methane Emission Inventory Recommendations." Prepared for WRAP by UNC-IE. February 2014. http://vibe.cira.colostate.edu/wiki/Attachments/Emissions/3SAQS_CH4_Emissions_Memo_Feb2014.pdf

Adelman, Z., U. Shanker, D. Yang and R. Morris. 2015. Three-State Air Quality Modeling Study CAMx Photochemical Grid Model Draft Model Performance Evaluation Simulation Year 2011. University of North Carolina at Chapel Hill and ENVIRON International Corporation, Novato, CA. June.

Boylan, J. W. 2004. "Calculating Statistics: Concentration Related Performance Goals", paper presented at the EPA PM Model Performance Workshop, Chapel Hill, NC. 11 February.

Boylan, J.W. and A.G. Russell. 2006. PM and Light Extinction Model Performance Metrics, Goals, and Criteria for Three-Dimensional Air Quality Models. Atmospheric Environment 40 (2006) 4946-4959.

Colella, P., and P.R. Woodward. 1984. The Piecewise Parabolic Method (PPM) for Gas-dynamical Simulations. *J. Comp. Phys.*, **54**, 174201.

ENVIRON and UNC. 2014. "Three-State Air Quality Study Phase 2 Scope of Work", prepared for WESTAR. University of North Carolina at Chapel Hill and ENVIRON International Corporation, Novato, CA.

ENVIRON. 2015. User's Guide Comprehensive Air-quality Model with extensions Version 6.2. ENVIRON International Corporation, Novato, CA. March. (http://www.camx.com/files/camxusersguide_v6-20.pdf).

EPA. 1991. "Guidance for Regulatory Application of the Urban Airshed Model (UAM), "Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency, Research Triangle Park, N.C. July. (http://www.epa.gov/ttn/scram/guidance/guide/uamreg.pdf).

EPA. 2007. Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5 and Regional Haze. U.S. Environmental Protection Agency, Research Triangle Park, NC. EPA-454/B-07-002. April. (http://www.epa.gov/ttn/scram/guidance/guide/final-03-pm-rh-guidance.pdf).

EPA. 2014. Draft Modeling Guidance for Demonstrating Attainment of Air Quality Goals for Ozone, $PM_{2.5}$ and Regional Haze. U.S. Environmental Protection Agency, Research Triangle Park, NC. December. (http://www.epa.gov/ttn/scram/guidance/guide/Draft_O3-PM-RH_Modeling_Guidance-2014.pdf).

EPA. 2015. Air Quality Modeling Technical Support Document for the 2008 Ozone NAAQS Transport Assessment. U.S. Environmental Protection Agency, Research Triangle Park, NC. January. (http://www3.epa.gov/airtransport/O3TransportAQModelingTSD.pdf)

EPA. 2015b. Technical Support Document, Preparation of Emissions Inventories for the Version 6.2, 2011 Emissions Modeling Platform. U.S. Environmental Protection Agency, Research Triangle Park, NC.

(http://www3.epa.gov/ttn/chief/emch/2011v6/2011v6_2_2017_2025_EmisMod_TSD_aug2015.pdf).

EPA. 2014a. Motor Vehicle Emissions Simulator (MOVES) – User Guide for MOVES2014. Assessment and Standards Division, Office of Transportation and Air Quality, U.S. Environmental Protection Agency. (EPA-420-B-14-055). July. (http://www.epa.gov/oms/models/moves/documents/420b14055.pdf).

EPA. 2014b. Motor Vehicle Emissions Simulator (MOVES) –MOVES2014 User Interface Manual. Assessment and Standards Division, Office of Transportation and Air Quality, U.S. Environmental Protection Agency. (EPA-420-B-14-067). July. (http://www.epa.gov/oms/models/moves/documents/420b14057.pdf).

EPA. 2014c. Motor Vehicle Emissions Simulator (MOVES) –MOVES2014 Software Design Reference Manual. Assessment and Standards Division, Office of Transportation and Air Quality, U.S. Environmental Protection Agency. (EPA-420-B-14-058). December. (http://www.epa.gov/oms/models/moves/documents/420b14056.pdf).

EPA. 2014d. Draft Modeling Guidance for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5 and Regional Haze. U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, RTP, NC. December 3. (http://www.epa.gov/ttn/scram/guidance/guide/Draft_O3-PM-RH_Modeling_Guidance-2014.pdf).

Guenther, A., X. Jiang, T. Duhl, T. Sakulyanontvittaya, J. Johnson and X. Wang. 2014. MEGAN version 2.10 User's Guide. Washington State University, Pullman, WA. May 12. (http://lar.wsu.edu/megan/docs/MEGAN2.1_User_GuideWSU.pdf).

Houyoux, M. R., C. J. Coats Jr., A. Eyth, and S. Lo, Emissions modeling for SMRAQ: A seasonal and regional example using SMOKE, paper presented at Computing in Environmental Resource Management, Air and Waste Manage. Assoc., Research Triangle Park, N. C., Dec. 2-4, 1996.

Houyoux, M.R., Vukovich, J.M., Coats Jr., C.J., Wheeler, N.J.M., Kasibhatla, P.S., 2000. Emission inventory development and processing for the Seasonal Model for Regional Air Quality (SMRAQ) project. Journal of Geophysical Research 105(D7), 9079-9090.

Mansell, G.E., S. Lau, J. Russell and M. Omary. 2006. Fugitive Wind Blown Dust Emissions and Model Performance Evaluation, Phase II, Final Report. ENVIRON International Corporation, Novato, CA. May 5. (http://www.wrapair.org/forums/dejf/documents/WRAP_WBD_PhaseII_Final_Report_050506.pdf).

McAlpine, JD, B. Brashers, R. Morris and K. Allen. 2014. WRF Meteorological Model Configuration for the BLM Montana/Dakotas Photochemical Grid Model Modeling Study. April, 2014.

Morris, R., C. Emery, J. Johnson and Z. Adelman. 2012. Technical Memorandum Number 12: Sea Salt and Lightning. ENVIRON International Corporation, Novato, California. June 25. (http://www.wrapair2.org/pdf/Memo_12_SeaSalt_Lightning_June25_2012_final.pdf).

NMED. 2007. Ozone Maintenance Plan for the Sunland Park, NM NAA. Air Quality Bureau New Mexico Environment Dept., Santa Fe, NM. (https://www.env.nm.gov/aqb/Control_Strat/sip/Sunland_MaintenancePlan.pdf).

Pouliot, G., H. Simon, P. Bhave, D. Tong, D. Mobley, T. Pace and T. Pierce. 2010. "Assessing the Anthropogenic Fugitive Dust Emission Inventory and Temporal Allocation Using an Updated Speciation of Particulate Matter", In Proceedings of the 19th International Inventory Conference, San Antonio, TX, September 27-30, 2010. (http://www.epa.gov/ttn/chief/conference/ei19/session9/pouliot.pdf).

Ramboll Environ and Systech Water Resources, 2015. A Case Study Assessment of Trace Metal Atmospheric Emissions and Their Aquatic Impacts in the San Juan River Basin. Phase 1: Four Corners Power Plant. Final Report. Prepared for R. Goldstein and L. Levin, EPRI. Novato, CA. September.

Simon, H., K. Baker and S. Phillips. 2012. Compilations and Interpretation of Photochemical Model Performance Statistics Published between 2006 and 2012. *Atmos. Env.* 61 (2012) 124-139. December. (http://www.sciencedirect.com/science/article/pii/S135223101200684X).

Skamarock, W. C. 2004. Evaluating Mesoscale NWP Models Using Kinetic Energy Spectra. *Mon. Wea. Rev.*, Volume 132, pp. 3019-3032. December. (http://www.mmm.ucar.edu/individual/skamarock/spectra_mwr_2004.pdf).

Skamarock, W. C., J. B. Klemp, J. Dudhia, D. O. Gill, D. M. Barker, W. Wang and J. G. Powers. 2005. A Description of the Advanced Research WRF Version 2. National Center for Atmospheric Research (NCAR), Boulder, CO. June. (http://www.mmm.ucar.edu/wrf/users/docs/arw_v2.pdf)

Skamarock, W. C. 2006. Positive-Definite and Monotonic Limiters for Unrestricted-Time-Step Transport Schemes. *Mon. Wea. Rev.*, Volume 134, pp. 2241-2242. June. (http://www.mmm.ucar.edu/individual/skamarock/advect3d_mwr.pdf).

UNC. "2010 Emissions Modeling Platform Spatial Surrogate Documentation." Prepared for U.S. EPA OAQPS by UNC-IE under contract EP-D-12-044, September 2013.

UNC and ENVIRON. "Three-State Air Quality Modeling Study – Final Modeling Protocol, 2008 Emissions & Air Quality Modeling Platform." 2013. http://vibe.cira.colostate.edu/wiki/Attachments/Modeling/3SAQS_2008_Modeling_Protocol_Final.pdf.

UNC and ENVIRON. "Three-State Air Quality Modeling Study – Final Modeling Protocol, 2011 Emissions & Air Quality Modeling Platform." 2014. http://vibe.cira.colostate.edu/wiki/Attachments/Modeling/3SAQS_2011_Modeling_Protocol_Finalv2.pdf.

UNC. 2008. Atmospheric Model Evaluation Tool (AMET) User's Guide. Institute for the Environment, University of North Carolina at Chapel Hill. May 30. (https://www.cmascenter.org/amet/documentation/1.1/AMET_Users_Guide_V1.1.pdf).

UNC. 2015. SMOKE v3.6.5 User's Manual. University of North Carolina at Chapel Hill, Institute for the Environment. (https://www.cmascenter.org/smoke/documentation/3.6.5/html/).

UNC and ENVIRON, 2015. Three-State Air Quality Modeling Study (3SAQS) – Weather Research Forecast 2011 Meteorological Model Application/Evaluation. University of North Carolina at Chapel Hill and ENVIRON International Corporation, Novato, CA. March 5. (http://vibe.cira.colostate.edu/wiki/Attachments/Modeling/3SAQS_2011_WRF_MPE_v05Mar2015.pdf).

Vukovich, J. and T. Pierce. 2002. "The Implementation of BEIS3 within the SMOKE Modeling Framework", In Proceedings of the 11th International Emissions Inventory Conference, Atlanta, Georgia, April 15-18, 2002. (http://www.epa.gov/ttn/chief/conference/ei11/modeling/vukovich.pdf).

Wiedinmyer, C., S.K. Akagi, R.J. Yokelson, L.K. Emmons, J.A. Al-Saadi, J.J. Orlando and A.J. Soja. 2011. The Fire Inventory from NCAR (FINN): a high resolution global model to estimate emission from open burning. Geosci. Moel. Dev., 4, 625-641. (http://www.geosci-model-dev.net/4/625/2011/gmd-4-625-2011.html).

Yarwood, G., J. Jung, G. Z. Whitten, G. Heo, J. Mellberg and M. Estes. 2010. Updates to the Carbon Bond Mechanism for Version 6 (CB6). 2010 CMAS Conference, Chapel Hill, NC. October. (http://www.cmascenter.org/conference/2010/abstracts/emery_updates_carbon_2010.pdf)

Zhang, L., S. Gong, J. Padro, L. Barrie. 2001. A size-segregated particle dry deposition scheme for an atmospheric aerosol module. *Atmos. Environ.*, **35**, 549-560.