APPENDIX I
PHOTOCHEMICAL MODELING PROTOCOL

Excerpted from:

South Coast AQMD 2022 Draft Air Quality Management Plan
Appendix V – Modeling and Attainment Demonstrations

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Background

One of the basic requirements of a modeling attainment demonstration is the development of a comprehensive modeling protocol that defines the scope of the regional modeling analyses. This includes the attainment demonstration methodology, meteorological and chemical transport platforms, gridded and speciated emission inventories, and geographical characteristics of the modeling domains. The protocol also defines the methodology to assess model performance and the selection of the simulation periods. The 2016 AQMP provided a comprehensive discussion of the modeling protocol used for the development of the PM2.5 and ozone attainment demonstrations. The 2016 AQMP Modeling Protocol served as the prototype of the 2022 AQMP modeling protocol. This AQMP demonstrates attainment of the 2015 federal 8-hour ozone standard with 2018 as the base year and 2037 as the attainment year. Future attainment years (See Table V-2-1) are identified based on nonattainment designation, pollutant standards, and geographical area.

TABLE V-2-1

UPCOMING ATTAINMENT YEARS FOR THE 2015 8-HOUR OZONE NAAQS

Attainment Year	NAAQS	NAAQS level	Areas
2018	Base Year	Modeling Base Year	
2026	2015 ozone	70 ppb	Ventura
2032	2015 ozone	70 ppb	Coachella, W. Mojave Desert
2037	2015 ozone	70 ppb	South Coast

Attainment Demonstration

8-hour Ozone

The 8-hour attainment demonstration was performed based on the U.S. EPA guidance document, “Modeling Guidance for Demonstrating Air Quality Goals for Ozone, PM2.5, and Regional Haze”, issued on November 29, 2018. The guidance requires that a maximum concentration be determined among 9 grid cells around a monitoring station and that the specific grid location be preserved in the future year modeling scenario when calculating relative response factors (RRF). The RRF calculation is limited to the top 10 days of simulated concentrations which are higher than 60 ppb. Focusing on the top 10 days produces future-year design values that are more responsive to emission reductions.

Numerical Models

Table V-2-2 provides a side-by-side comparison of the 2012, 2016 and the current 2022 AQMP modeling protocols. In general, changes have occurred in the following categories: emissions inventories, future-year simulations, the level of the non-attainment designation and the attainment demonstration methodology. As such, these changes are expected to occur with each subsequent modeling update. Table V-2-3 highlights the main differences in CMAQ setup since the 2016 AQMP.

TABLE V-2-2

NUMERICAL MODELING PLATFORMS AND DOMAINS FOR 2022 AND PREVIOUS AQMPS

	2012 AQMP	2016 AQMP	2022 AQMP
Modeling Base Year	2008 Ozone: June – Aug PM: Annual	2012 Ozone: May – Sep PM: Annual	2018 Ozone: May - Sep
Chemical Transport Model	CMAQ as primary tool CAMx as weight of evidence	CMAQ	CMAQ
Meteorological Model	WRF version 3.3 with Updated Land Use	WRF version 3.6 with Updated Land Use	WRF version 4.0.3 Unified Noah
Emission: On-Road Off-Road	EMFAC 2011 EMFAC-LDV EMFAC-HD EMFAC-SG Category Specific Calculation	EMFAC 2014 Single package Category Specific Calculation	EMFAC 2017 Single package Category Specific Calculation
Modeling Domain	624 km by 408 km	624 km by 408 km	624 km by 408 km
Grid Resolution	4km by 4 km grid	4km by 4km grid	4km by 4km grid
Vertical Layer	18 layers with 14 layer below 2000 m Above Ground Level (AGL) and 50 hPa as top boundary	18 layers with 14 layer below 2000 m AGL and 50 hPa as top boundary	30 layers with 14 layer below 2000 m AGL and 50 hPa as top boundary

TABLE V-2-3

CHEMICAL TRANSPORT MODELING PLATFORM FOR THE 2016 AND 2012 AQMPS

Options	2016 AQMP	2022 AQMP
Numerical Model	CMAQ version 5.0.2	CMAQ version 5.2.1
Modeling Grid	156 by 102 grids with 4 km grid distance	Same
Vertical Layers	18 layers	30 layers
Gas Phase Chemical Mechanism	SAPRC07 with version "c" toluene updates	Same
Aerosol Mechanism	AERO6	Same
Chemical Solver	Euler Backward Iterative solver (EBI)	Same
Horizontal Advection	Yamo	Same
Vertical Advection	WRF	Same
Horizontal Diffusion	Multiscale CMAQ scheme	Same
Vertical Diffusion	ACM2	Same
Photolysis	In-line Calculation	Same
Initial Values	Clean Homogeneous Condition	Same
Boundary Values	Model for OZone and Related chemical Tracers (MOZART)	Nested modeling with 12km statewide CMAQ The Outer CMAQ domain used boundaries from the global model of Community Atmosphere Model with Chemistry (CAM-chem)

The Weather Research and Forecast (WRF) model remains the primary tool for meteorological modeling. WRF was updated with the most recent version (version 4.0.3) available at the time of protocol preparation and was evaluated with a set of observation data. Later WRF version 4.3 was conducted and evaluated to ensure the accuracy and reliability of meteorological predictions, while version 4.0.3 served as the primary WRF for this AQMP. WRF simulations were conducted with three nested domains with grid resolutions of 36, 12 and 4 km. The innermost domain spans 652 km by 460 km in the east–west and north–south directions, respectively, which includes the greater Los Angeles area, its surrounding mountains, and ocean waters off the coast of the Basin (Figure V-2-1). A Lambert conformal map projection was used with reference latitudes of 30° and 60° N and the center of the modeling domain positioned at 37° N and 120° 30’ W. Details on the WRF model configuration are provided in Chapter 3.

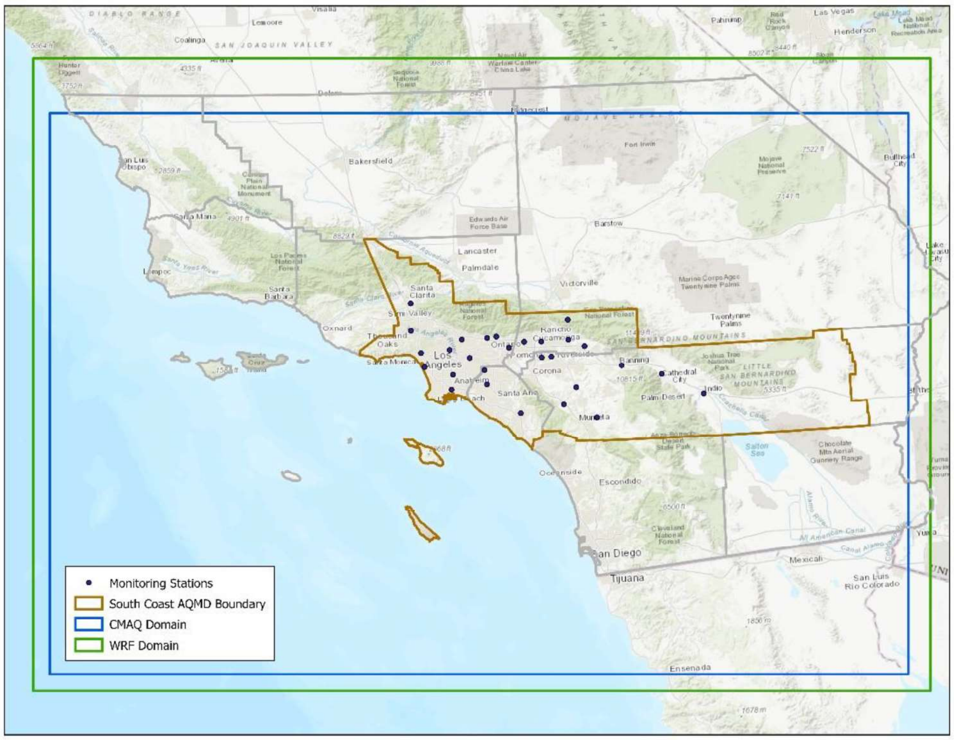

FIGURE V-2-1

THE RELATIVE LOCATIONS OF THE INNER MOST WRF DOMAIN COMPARED TO THE CMAQ DOMAIN. THE BOUNDARY OF SOUTH COAST AQMD JURISDICTION BOUNDARY AND AIR MONITORING LOCATIONS ARE OVERLAID BY A THICK SOLID LINE AND BLACK DOTS, RESPECTIVELY.

Emissions Processing

Emissions inventories are often developed on an annual basis for large geographic areas and a process must be developed to allocate the emissions to a time-dependent grid for use in chemical transport modeling. Traditionally, emissions were allocated to the modeling grid using generic or average activity patterns and profiles. These approaches did not sufficiently reflect the real-world characteristics of emissions sources. Shortcomings of previous emissions allocation methods included an inability to account for traffic flows responding to changes in weather, vessels transiting outside of well-known shipping lanes, or aircraft following airport-specific landing and takeoff trajectories. For these reasons, new approaches were developed to spatially and temporally allocate emissions from on-road mobile sources, Ocean-Going Vessels (OGV), and aircraft. Each method used information from sensor or transponder-based datasets, which accurately reflected where and when emissions were occurring. Further details on the updated allocation methods are presented in Chapter 4 of this appendix.

TABLE V-2-4

SUMMARY OF EMISSION PROCESSING FOR 2016 AND 2022 AQMPS

Options	2016 AQMP	2022 AQMP
On-Road Emissions	EMFAC 2014 ○ Emissions mode to get total amount of emissions in Tons per Day ○ Emissions rate to estimate grams per emissions of specific vehicle category, activity, etc.	EMFAC 2017
	Temporal allocation using Caltrans real-time Performance Measurement System (PeMS) traffic data for light and medium duty vehicles, and Weight in Motion (WIM) for heavy duty vehicles	Temporal allocation using Caltrans real-time PeMS single loop detector-based traffic data for light, medium, and heavy-duty vehicles
Aircraft Emissions	Treated as point sources with inline emissions calculation	ACARS/GATE[1] spatial allocation
OGV Emissions	Prescribed spatial allocation following major shipping channels	AIS-based[2] spatial allocation
Vehicle Miles Traveled	2016 Regional Transportation Plan/Sustainable Communities Strategy (RTP/SCS)	2020 Regional Transportation Plan/Sustainable Communities Strategy (RTP/SCS)
Off-Road Emissions	Category Specific Calculation	Same
Mexico Emissions	CARB's Mexican emissions profile	Same

[1] Aircraft Communication Addressing and Reporting System (ACARS)/Gridded Aircraft Trajectory Emissions (GATE)

[2] Automated Identification System

TABLE V-2-5

LIST OF EMISSIONS CATEGORIES WITH AND TEMPORAL PROFILE USED

Day-Specific Profile	Generic Profile
• Wildfires[1] • Prescribed burns[1] • Biogenic and On-Road motor vehicle emissions are adjusted using day/hour-specific meteorological data.	• Agricultural burning • Residential wood combustion • Facilities • Paved road dust • Unpaved road dust • Windblown dust • Livestock dust

[1] Wildfires and prescribed burns were modeled using day-specific profiles for the model performance evaluation only. For the attainment demonstration, wildfire emissions were excluded, and prescribed burns were modeled using a generic profile.

V-2-Biogenic Emissions

Daily biogenic VOC emissions were calculated using the Model of Emissions of Gases and Aerosols from Nature version 3.0 (MEGAN3.0) using 2018 meteorology as input. MEGAN was executed in its default configuration, except for the normalized Leaf Area Index (LAIv) input. LAIv was developed by the California Air Resources Board using 2018 data from the Moderate Resolution Imaging Spectroradiometer (MODIS) on the National Aeronautical Space Administration's Terra and Aqua satellites. Because MODIS does not provide data in urban areas, LAIv in these areas was based on tree survey data from the US Forest Service. A detailed description of the biogenic inventory is provided in Chapter 4.

Computational Resources

The main computation platform employs high performance nodes. New servers, compiled to enhance computational capability, were configured with Red-Hat Enterprise Linux 7 and 64-bit operating systems. Details of the computing resources are summarized in Table V-2-6.

TABLE V-2-6

DETAILS OF COMPUTATIONAL RESOURCES USED IN THE 2012, 2016 AND 2022 AQMPS.

2012 AQMP	2016 AQMP	2022 AQMP
HP DL380 G7, 64 bit 3.3 GHz, 2x6 cores	HP DL560 G8, 64 bit 4x8 cores	HP DL380 G10, 64 bit 2x16 cores
HP DL560 G8 Total **140** processors	HP DL560 G8, Total **320** processors	HPE DL380 G10 Total **320** processors
	HP DL560 G8 Total **64** processors	HP DL560 G8, Total **256** processors

References

US EPA (2018) Modeling Guidance for Demonstrating Air Quality Goals for Ozone, PM2.5, and Regional Haze