Evaluation of the Community Multiscale Air Quality (CMAQ) modeling system version 5.3.3 over California: Preliminary Analysis

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Introduction/Background

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The Community Multiscale Air Quality (CMAQ) model is U.S. EPA's open-source regional photochemical model widely used in the regulatory and scientific communities and represents the current state-of-the-science. CMAQ version 5.3.3 (Appel et al., 2021) was released to the public in August 2021 and has numerous scientific updates* when compared to previous versions including but not limited to:

(1) Improved representation of O_3 dry deposition to snow
(2) A new deposition module – the Surface Tiled Aerosol and Gaseous Exchange (STAGE) model is incorporated to estimate land-use specific deposition
(3) Updated aerosol module (AERO7) that explicitly tracks 84 particulate species
(4) Updated pathways for secondary organic aerosol formation from biogenic VOCs
(5) Harmonized treatment of water uptake to aerosol organic phase to improve representation of aerosol chemistry, mixing state, and optical properties
(6) Improved the representation of bi-directional exchange of ammonia at the surface
(7) Updated marine chemistry to represent impacts of (1) halogen chemistry on ozone depletion and sulfate formation and (2) dimethyl sulfide on aerosol sulfate
(8) Expanded the representation of secondary pollutant formation in clouds (AQCHEM-KMT2).

* https://github.com/USEPA/CMAQ/tree/master/DOCS/Release_Notes

In this poster, we present preliminary findings from an ongoing evaluation of the CMAQ533 modeling system comprised of the Weather Research Forecasting v4.2.1 (WRF421) and the Sparse Matrix Operator Kernel Emissions 4.8 (SMOKE48) over California with a focus on the South Coast Air Basin. The US EPA's Atmospheric Model Evaluation Tool (Appel et al., 2018) was used for evaluating the WRF and CMAQ model performance in this study.

WRF Meteorological Model Configuration

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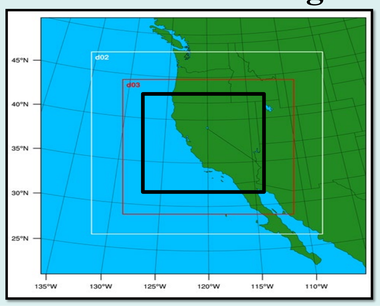

WRF modeling domains (D01 36km; D02 12km; and D03 (427x427) 4km. CMAQ simulations for this study were conducted using the 4 km inner modeling domain (black box) that covers the entire California.

Key WRF Physics Options

Physics Option	
Microphysics	WSM 6-class
Longwave Radiation	RRTM
Shortwave Radiation	Dudhia
Surface Layer	Revised MM5 Monin-Obukhov
Land Surface Model	Pleim-Xu look-up table LSM
Planetary Boundary Layer	YSU
Cumulus Parameterization	Kain-Fritsch Scheme (for D01 and D02 only)

- Meteorology Model: WRF version 4.2.1
- Modeling Period: June 20 – July 31, 2017
  - Three-nested domains 36-km (D01), 12-km (D02), and 4-km (D03)
  - The 4-km innermost domain (d03 in red) has 427x427 grid points and spans 1748 km in the east-west and the north-south direction.
  - 30 vertical layers with the lowest layer extending to 30 m above the surface.
- The North America Regional Reanalysis (NARR) fields (32 km), were used for initial and boundary conditions (IC/BCs) and updated every 6 hours
- The IC/BCs were further refined with surface and upper air observations obtained from the National Center for Atmospheric Research (NCAR)
- Four Dimension Data Assimilation (FDDA) was applied only on the outermost (36-km) domain.
- WRF was reinitialized every 6 days with one day overlap, where the first day after reinitialization was discarded as model spin-up

WRF Model Performance Statistics: July 2017

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Model performance statistics for various meteorological variables simulated by WRF

Parameter	2m Temperature (K)	2-m Mixing Ratio (kg/kg)	10-m wind speed (m/s)	10-m wind direction
Number of data points	155438	154083	117015	117015
Correlation	0.93	0.67	0.48	n/a
Mean Bias	-1.2	1.75	1.47	48.66
Mean Error	2.47	0.51	-0.79	1.65
Normalized Mean Bias (%)	-0.40	5.86	-20.87	n/a
Root Mean Squared Error (%)	3.17	2.39	2.01	67.32
Index of Agreement	0.92	0.65	0.44	n/a

Note: The statistical metrics shown in this table were generated using the Atmospheric Model Evaluation Tool (AMET) and MADIS observations https://madis.ncep.noaa.gov/index.shtml

CMAQ Model Configuration

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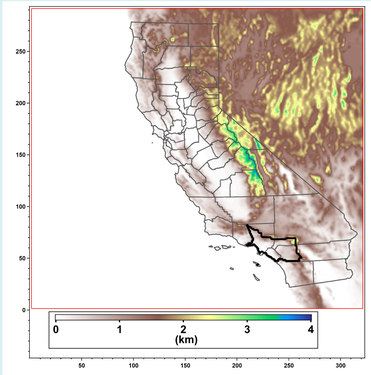

The spatial extent (red box) of 4km CMAQ modeling domain (321x291 grid cells) that covers entire California. The shaded and black line contours denote the gradients in topography (km) and the regional boundary of California's South Coast (SC) Air Basin.

Key CMAQ Simulation Settings

- Domain: 321x291 grid cells with 4km horizontal resolution
- MCIPv5.1 with 30 vertical levels
- Modeling Period: July 2017 with 1-week (June 24 – June 30) spin up
- Anthropogenic emission inventory: CARB's Day-specific 2017 gridded modeling inventory
- Biogenic emission inventory: MEGAN 3.0 model
- Boundary conditions: CAM-Chem global model output

The performance of CMAQ533, using the State Air Pollution Research Center version 07tc with extended isoprene chemistry (SAPRC07tic) and aerosol module (AERO6) treatment for SOA, was evaluated by comparing simulated ozone values to: (1) similarly configured CMAQv521 (Appel et al., 2017); (2) v533 with new aerosol module (AERO7); (3) v533 with STAGE dry deposition model. The key CMAQ settings are summarized in the table below.

Simulation Name	CMAQ version	Chemical Mechanism	Deposition Model
v521_AE6	v521	saprc07tic_ae6i	M3Dry
v533_AE6	v533	saprc07tic_ae6i	M3Dry
v533_AE7	v533	saprc07tic_ae7i	M3Dry
v533_AE7_STAGE	v533	saprc07tic_ae7i	STAGE

Evaluation of Daily Maximum 8-hour (MDA8) ozone in South Coast for July 2017

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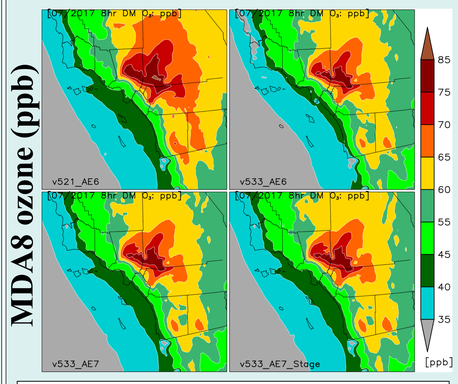


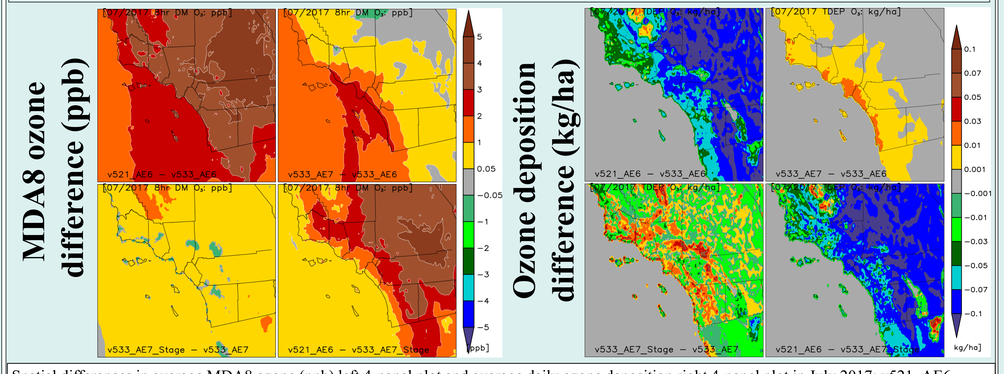
Spatial distribution of averaged July 2017 MDA8 ozone (ppb) for CMAQ simulation with v521_AE6 (top left), v533_AE6 (top right), v533_AE7 (bottom left) and v533_AE7_STAGE.

Daily Maximum 8-hour Average ozone model performance Statistics for July 2017 in SC

Parameter	v521_AE6	v533_AE6	v533_AE7	v533_AE7_STAGE
Number of data points	878	878	878	878
Correlation	0.75	0.75	0.74	0.74
Mean Bias (ppb)	-1.07	-4.68	-3.33	-2.96
Mean Error (ppb)	11.6	12	11.9	11.9
Normalized Mean Bias (%)	-1.67	-7.32	-5.21	-4.64
Root Mean Squared Error (%)	14.6	15.3	15.2	15.1
Index of Agreement	0.83	0.82	0.81	0.82

Note: The statistical metrics shown in this table were generated using Atmospheric Model Evaluation Tool (AMET) and EPA's AQS ozone observations

The CMAQ simulations match the AQS observations well with a negative bias (~ -1 to -5 ppb) and capture the broad spatial patterns (4-panel plot above) in ozone with enhanced values over Los Angeles region. Within the CMAQv533 framework, the AERO7 module produces higher ozone than AERO6 along the coast (top right panel of MDA8 ozone difference 4-panel spatial plot). The simulated values are generally lower with CMAQv533 when compared to CMAQv521 (top left panel of the MDA8 ozone difference 4-panel spatial plot) by ~ 3-5 ppb on average, which could be partially attributed to differences in the total deposition of ozone (top left and bottom right panels of the ozone deposition difference 4-panel spatial plot).



Spatial differences in average MDA8 ozone (ppb) left 4-panel plot and average daily ozone deposition right 4-panel plot in July 2017: v521_AE6 – v533 AE6 (top left), v533_AE7-v5333_AE6 (top right), v533_AE7_Stage – v533_AE7 (bottom left) and v521_AE6- v533_AE7_STAGE simulations.

Temporal variability of MDA8 ozone in South Coast (SC) for July 2017

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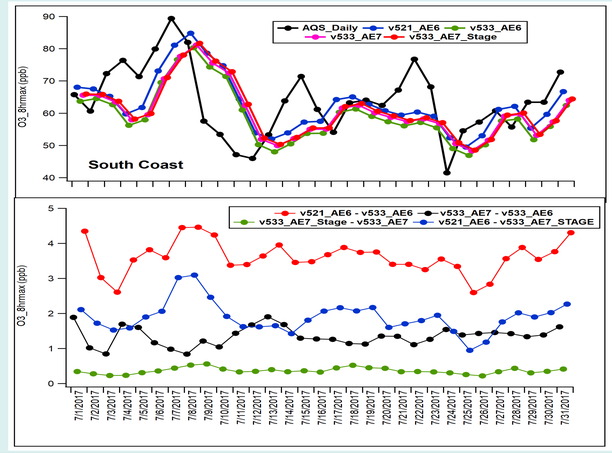
The temporal variability in the MDA8 ozone were analyzed by comparing the time series of modeled MDA8 ozone with observations averaged over SC (below). CMAQv533 generally produces less ozone compared to CMAQv521 (~3.5 ppb). Within the CMAQv533 framework, the AE7 module produces higher ozone when compared to AE6, which is consistent with the spatial distribution of averaged July 2017 MDA8 ozone shown earlier.



Timeseries of observed (black) and simulated MDA8 ozone (ppb) averaged over 29 sites in South Coast region for July 2017 (top panel): v521_AE6 (blue), v533_AE6 (green), v533_AE7 (magenta), v533_AE7_STAGE (red).
The bottom panel shows the differences in MDA8 ozone for v521_AE6 – v533 AE6 (red), v533_AE7-v533_AE6 (black), v533_AE7_Stage – v533_AE7 (green) and v521_AE6-v533_AE7_STAGE (blue) simulations.

Summary and Preliminary findings

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- CMAQv533 is able to simulate the broad spatial patterns and temporal variability in ozone over the South Coast region but the simulated values are generally lower with CMAQv533 (~ 3.5 ppb on average) when compared to CMAQv521
- Within the CMAQv533 framework: AE7 and STAGE dry deposition produce ~ 1.5 pb and 0.5 ppb average difference in MDA8 in the SC region

Ongoing and Future work

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- The MDA8 ozone analysis is currently ongoing for other air basins including San Joaquin Valley and Sacramento Metropolitan Areas for the CMAQ simulations in this poster
- Study the impact of AE7 and STAGE deposition modules on $PM_{2.5}$ species and other species including NO_x, Nitrate and monoterpene SOA
- Analyze the December 2017 modeling simulations to study the impact of AE7 and STAGE deposition on wintertime ozone and $PM_{2.5}$
- Repeat the July 2017 CMAQ simulations to output diagnostics deposition output including the deposition velocities to further understand the impact of deposition updates on simulated ozone and $PM_{2.5}$
- Study the impact of non-volatile and semi-volatile POA options on $PM_{2.5}$
- Extend this analysis to seasonal and annual modeling simulations to study the seasonal differences in ozone and $PM_{2.5}$

References

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Acknowledgments

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