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Diagnostic and Mechanistic Evaluations of MM5-CMAQv4.6 for the Summer 2000 Central California Ozone Study

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1. Abstract

Past evaluations of Community Multiscale Air Quality (CMAQ) modeling system have focused on the eastern United States and applications of it are usually conducted for high ozone episodes that last for a few days. In our research, we seek more comprehensive model evaluation by applying MM5-CMAQ to simulating ozone formation for an entire summer season contained in the 2000 Central California Ozone Study. Ozone air pollution problems are severe in the central California region and air districts are out of compliance with the 8-hour ozone standard.

In this study, we apply CMAQ (version 4.6) to a 15-day period that contains a high ozone episode in the middle 5 days as well as relative low ozone days before and after that. Model parameters and inputs are set to reflect actual conditions of the modeling domain. We apply a variety of evaluation and diagnostic methods to assess model performance across a range of days and locations, with significant spatial and temporal variations in air quality. Effects of meteorological data assimilation are evaluated. We perform sensitivity analyses with the brute force method and Direct Decoupled method (DDM) to diagnose causes for discrepancies between observations and model predictions.

2. Air Quality in Central California

- Topography and meteorology give rise to large pollutant loadings. San Francisco Bay forms a gap in the coastal range that allows wind to blow pollutants into valley from other regions.
- Region is seriously out of attainment with previous and current ozone standards.
- Potential to get worse because it is one of the fastest growing areas with increased human activity and land use changes (urbanization)

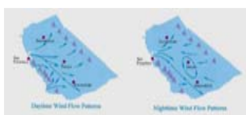


Figure 1 Geography of the modeling domain.
SJV: San Joaquin Valley
SV: Sacramento Valley
SFB: SF Bay Area
SCC, NCC: South and North Central Coast

Figure 2 Central California wind patterns during ozone season (source: "San Joaquin Valley Air Basin Plan Demonstrating Attainment Of Federal 1-hour Ozone Standards", by San Joaquin Valley Air Pollution Control District, October 8, 2004.)

3. CMAQ Modeling System

- 5-day ozone episode:
  Jul 29th – Aug 2nd, 2000
  15-day period:
  Jul 24th – Aug 8th, 2000
- SARMAP domain: 4 km by 4 km grid , 27 layers (~17 km).
- CMAQ4.6 EBI solver and SAPRC99 chemical mechanism
- Adjusted parameters:
  - Ozone dry deposition velocity over the ocean is set to 0.04 cm/s
  - Minimum eddy diffusivity is set to 0.1 m/s
- Initial conditions: 3-day spinup
- Boundary conditions: vertically varying profiles adapted from observations and literature
- Day-variable model inputs
  - Met (15 day): MM5 non-FDDA
  - Met (mid 5 day): MM5 FDDA
  - Emissions:
    - Day specific mobile source and area sources
    - Date specific biogenic and point sources

4. Model Simulation and Evaluation

- Model correctly predicts higher ozone in the 5-day episode (Figure 3), but underpredicts peaks.
- Model produces reasonable ozone spatial trend (Figure 4).
  - Lower on coastal and mountain areas and higher in the Central Valley and SFB

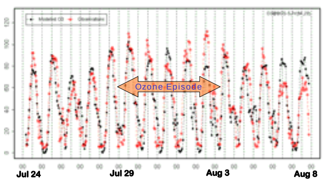


Figure 3 Time series of predicted and observed ozone mixing ratios (ppb) vs. time (hr PST) at Bakersfield in SJV

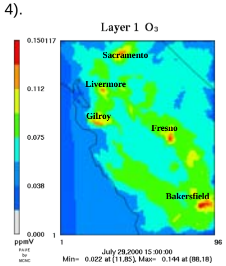


Figure 4 **Predicted ozone mixing ratios at 3pm on Jul 29th 2000.**

Table 1 Evaluation and Diagnostic Methods

Method	Usage
Taylor Diagram (correlation, standard deviation, and root mean squared difference)	Describe how well patterns in modeled and observed values match each other
Mean Bias	Average sign in model prediction errors
RMSE, Gross Error	Magnitude of model prediction errors
Spatial Krigging	Spatial variation in model performance
Ozone Production Efficiency (O_x v.s. NO_2)	Compare limiting regimes presented in the observed and modeled air masses
Sensitivity Analysis (Decoupled Direct Method, Brute Force Method)	Identify the influential parameters that affect model performances

4.1 Temporal Trend in Model Performance

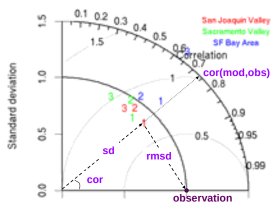


Figure 5 Taylor diagram showing daytime **pattern statistics** *normalized by observed standard deviation*, for July 24-29 (**1**), July 29-August 2 (**2**), August 2-7 (**3**), respectively, at three air basins.

cor: correlation between observed and modeled ozone

sd: standard deviation; rmsd: root mean squared difference. The closer to **observation** point (sd→ 1, and cor→1, rmsd→0), the better model performance.

Table 2 Summary statistics for three 5-day periods

	Normalized Bias			Normalized Gross Error		
	1	2	3	1	2	3
1h Peak O_3	-10%	-7%	-4%	17%	20%	18%
8h Peak O_3	-15%	-12%	-11%	17%	17%	18%
Daytime NO_x	0%	-4%	3%	57%	60%	64%
Nighttime $NO_2 + O_3$	8%	10%	8%	19%	29%	22%

Peak ozone cutoff value: 60 ppb, NOx and Ox: 10 ppb.

- Overall, pattern statistics indicate similar model performance over the three 5-day periods, except SF Bay area.
- Gross error indicates better performance in predicting ozone than its precursors. Model underpredicts peak ozone.
- No significant numerical error accumulation indicated by biases or gross errors.

4.2 Spatial Trend in Model Performance

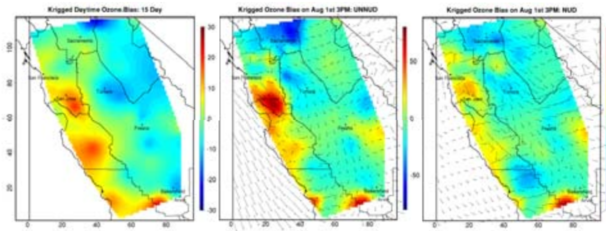


Figure 6 Spatial distribution of ozone biases. From left to right : average daytime ozone bias over the 15-day period; ozone bias at 3 PM on Day 214 with unnudged and nudged wind fields. Surface wind averaged from 1-3PM is plotted.

- Model overpredicts ozone along the western coastal areas. Biases are generally larger near the boundaries.
- Four dimensional wind nudging produces most noticeable improvements on Aug 1st, where ozone biases are also reduced by a factor of two.

4.3 Ozone Production Efficiency

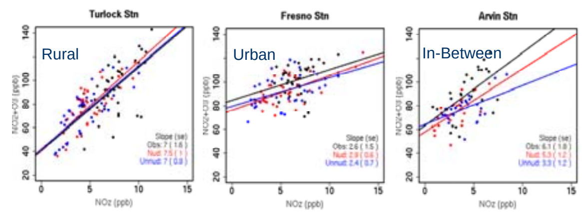
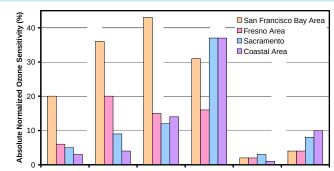


Figure 7 Ozone production efficiency (the linearly fitted slope) at three sites evaluated for observed and modeled (with and without wind nudging) daytime data during weekdays in the middle 5-day period.

4.4 Sensitivity Analysis



- SF Bay area is sensitive to both anthropogenic and biogenic emission sources, as well as boundary O_3 , while Fresno is more sensitive to anthropogenic emissions.
- Boundary O_3 significantly affects all the nearby areas

Figure 8 O_3 sensitivity at various locations to emissions of biogenic VOC (O_3_BVOC), anthropogenic VOC (O_3_AVOC), NO_x (O_3_NO_x), boundary NO_y (O_3_BCNO_y), boundary O_3 (O_3_BCO_3), and boundary VOC (O_3_BCVOC).

5. Conclusions

CMAQ performance in central California region does not differ significantly between high and low ozone periods, except for the SF Bay area. Model tends to over predict ozone along the coastal areas. Wind nudging improves chemical transport processes and results in more accurate localization of ozone plumes. Modeled and observed ozone production efficiencies are similar when transport errors are reduced by wind nudging. The Bay area is highly sensitive to uncertainties in all the emission sources as well as boundary conditions, which suggests great challenges on correct simulating ozone concentrations in this area.

Acknowledgement

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