Ozone Simulation During CABOTS Period

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Goal

• Simulate Base-case ozone
• Evaluate and improve model performance
• Investigate ozone reductions from planned and adopted emission controls?
• Investigate relative contributions of locally generated vs transported ozone
• Quantify intercontinental ozone transport
Ozone Simulation

Presentation:
• Emissions inventory preparation: Jeff Matsuoka
• Meteorological simulation: Yiqin Jia
• Air quality simulation: Steve Soong

CABOTS Modeling Domain, the same as CCOS/CRPAQS domain
Emissions Inventory Preparation

Geographic Extent

- Same domain as 2000 Central California Ozone Study (CCOS)
- 185 x 185, with 4km x 4km grid resolution
- No Nevada emissions
Sources of Emissions Data

- Downloaded 2016 data which ARB developed for Ozone SIP
- Supplemented with detailed point source information from BAAQMD permit data
  - Used CCOS detailed information for point sources outside Bay Area
- Biogenic emissions from CCOS (2000) ARB inventory, adjusted for Temperature
  - Evaluating MEGAN, BEIS3
SMOKE Model

- US EPA emissions processing model
- Prepares spatially allocated, chemically speciated hourly emissions for direct input into CMAQ
- Generates custom reports for QA/QC
Bay Area 2016 Annual Average Anthropogenic Emissions

<table>
<thead>
<tr>
<th>2016 (tons per day)</th>
<th>CO</th>
<th>NOX</th>
<th>SO2</th>
<th>TOG</th>
<th>NH3</th>
<th>PM2.5</th>
<th>PM10</th>
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<tr>
<td>Area</td>
<td>76.2</td>
<td>20.9</td>
<td>0.5</td>
<td>244.1</td>
<td>19.5</td>
<td>20.3</td>
<td>61.3</td>
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<tr>
<td>Nonroad</td>
<td>359.2</td>
<td>120.1</td>
<td>3.4</td>
<td>48.4</td>
<td>0.1</td>
<td>4.3</td>
<td>4.8</td>
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<tr>
<td>Mobile</td>
<td>335.0</td>
<td>95.8</td>
<td>0.7</td>
<td>47.9</td>
<td>5.5</td>
<td>4.7</td>
<td>10.0</td>
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<td>Stationary</td>
<td>29.3</td>
<td>33.8</td>
<td>21.3</td>
<td>222.6</td>
<td>5.0</td>
<td>8.6</td>
<td>12.8</td>
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<tr>
<td>TOTAL</td>
<td>799.7</td>
<td>270.6</td>
<td>26.0</td>
<td>563.0</td>
<td>30.1</td>
<td>37.8</td>
<td>88.9</td>
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Total Processed Emissions by Region
Sept. 26, 2016

<table>
<thead>
<tr>
<th>Region</th>
<th>NOX</th>
<th>ROG</th>
<th>PM2.5</th>
<th>NH3</th>
<th>CO</th>
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<tr>
<td>Bay Area</td>
<td>254</td>
<td>250</td>
<td>34</td>
<td>33</td>
<td>275</td>
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<tr>
<td>Sac Valley</td>
<td>250</td>
<td>616</td>
<td>22</td>
<td>23</td>
<td>275</td>
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<tr>
<td>S. Joaquin</td>
<td>275</td>
<td>1,145</td>
<td>61</td>
<td>314</td>
<td>458</td>
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</table>
Distributions of ROG and NOx emissions
Sept. 26, 2016
Summary

- Emissions data were mainly obtained from ARB Ozone SIP inventory.
- The SMOKE model was used to process annual average county-level emissions into CMAQ model-ready format for May 15 – Oct 15, 2016.
- Future improvements: biogenic emissions, update detailed point source information outside Bay Area
Meteorological Modeling

WRF Modeling Basics

• WRF version 3.8
• CCOS/CRPAQS domain:
  • Three nested domains: 36km (91x95); 12km (157x151); 4km (190x190)
  • 4km domain covers central and portions of northern California
• NCEP North America Mesoscale (NAM) 12 km Analysis was used as the first guess input
• NCEP ADP Global Surface and Upper Air Observational Weather Data were used for objective analysis
WRF Configuration -- Physics

• Morrison (two moments) microphysics (mp_physcis = 10)
• RRTM short and long wave radiation scheme (ra_lw_physics=4)
• Multi-scale Kain-Fritsch cumulus scheme (cu_physics=11)
• Noah Land Surface Model (sf_surface_physics=2)
• YSU PBL scheme (bl_pbl_physics=1)
• Single-layer urban canopy model (sf_urban_physics=1)

Some of the selected options have been rigorously tested
WRF Configuration -- FDDA Options

• Surface Analysis FDDA was on the 36 and 12 km domains with 3-hourly interval
• 3-D Analysis FDDA was on the 36 and 12 km domains with 6-hourly interval
• No boundary FDDA of temperature and humidity; observation FDDA of wind only

These options also have been previously tested
Structure of Mass Production Run

• May to October, 2016
• Five-day chunk with one day overlapped between each chunk
• An example for a month long run (start dates and hours):
  2016-05-01_12, 2016-05-05_12, 2016-05-09_12, 2016-05-13_12,
  2016-05-17_12, 2016-05-21_12, 2016-05-25_12, 2016-05-29_12
Model Evaluation

- Observations used: AQS, BAAQMD Met Network, NCDC observation and CABOTS Ozonesonde data
- Sample METSTAT statistics

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<tbody>
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<td>-0.33</td>
<td>-0.18</td>
<td>0.18</td>
<td>-0.06</td>
<td>-0.75</td>
<td>-0.74</td>
<td>-0.68</td>
<td>-0.04</td>
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<td>1.12</td>
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<td>1.75</td>
<td>1.64</td>
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<td>0.73</td>
<td>0.69</td>
<td>0.72</td>
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<td>0.81</td>
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<td>Humidity RMSE</td>
<td>1.49</td>
<td>1.48</td>
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<td>1.39</td>
<td>0.82</td>
<td>0.78</td>
<td>0.61</td>
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<td>0.62</td>
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<td>0.54</td>
<td>0.5</td>
<td>0.8</td>
<td>0.7</td>
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Model Evaluation – Hourly Time Series at Livermore
Model Evaluation -- Oakland Sounding, June 3, 2016
Solid – Observation; Dash -- Simulation
Model Evaluation – Bodega Bay Ozonesonde, June 3 -4, 2016

Temperature at Bodega Bay at 21GMT on June 3, 2016

- Temperature at Bodega Bay at 21GMT on June 4, 2016
Future Work

• Sensitivity test on Land Surface Model (LSM) and PBL scheme: Pleim-Xiu & ACM2
• Sensitivity test on Land Use Categories: USGS24, MODIS21, or NLCD40
• Obtain feedback from CMAQ performance for different WRF meteorological inputs, adjust and finalize the WRF configurations
• Conduct additional model evaluation and analysis
CMAQ Base-case Specifications

- Domain: Same as the CCOS domain
  - Horizontal resolution: 4 km
  - Vertical resolution: 15 layers, lowest layer thickness - 32 m
- CMAQ version: 5.1
- Chemical Mechanisms: SAPRC07 AE6
- Initial and Lateral Boundary Conditions: MOZART
- WRF runs: Noah LSM
CMAQ Domain and Example of Simulated O3
23 UTC September 26, 2016
Simulated and Observed 1-Hour O3
SFB Area Average

SFB Area Average 1 HR Ozone
May 15 - Oct 15 2016

O3 (ppb)
Effect of WRF LSM on Simulated O3
Noah (base) vs Pleim-Xiu (PX) LSM

Effect of Model Variations on CMAQ Simulated O3
Sep 22-29, 2016
Effect of CMAQ Versions on Simulated O3
CMAQv5.1 vs CMAQv5.0.2

Effect of Model Variations on CMAQ Simulated O3
Sep 22-29, 2016
Effect of Lateral Boundary Condition on Simulated O3

- Half Moon Bay and Mozart O3 sounding comparison
- Effect of Half Moon Bay O3 sounding on simulated O3
- Effect of 10 ppb lateral boundary error on simulated O3
- Effect of 10 ppb lateral boundary error in selected layers on simulated surface O3
Half Moon Bay O3
Mozart Simulation vs Observation

SJSU Observed Ozone and Mozart Ozone Averaged over 07-15 to 08-17, 2016
Half Moon Bay
Effect of Lateral Boundary O3 on SFB Area Average O3
Effect of 10 ppb Lateral Boundary O3 error on SFB Area Average O3
Effect of 10 ppb Lateral Boundary O3 error in Selected Layers on SFB Area Average O3
Conclusions

• CMAQ base case simulation using WRF Noah LSM meteorology underestimated O3 in the SFB Area
• CMAQ simulation using WRF Pleim-Xiu LSM meteorology produced better results
• Mozart BCs resulted in O3 underestimates of as much as 15 ppb below 8 km
• Lateral boundary O3 error had large effect on simulated O3 in the SFB Area
• Lateral boundary O3 error in the 1-2 km layer had the largest effect on simulated O3 in the SFB Area for September 22-29, 2016