Air Quality Uncertainties: Choosing among chemical mechanism, meteorology, and model

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CESM Chemistry Climate Working Group Session
Thursday, June 23, 2016
Overview

Research Questions:

What is the impact of the choice of chemical mechanism, model, meteorology, and resolution on surface chemistry (i.e. O3 and PM2.5 biases)?

What configuration(s) is (are) the most efficient for human health impact studies? Does this answer depend on region?

<table>
<thead>
<tr>
<th>Emissions</th>
<th>Meteorology</th>
<th>Mechanism</th>
<th>Abbreviation</th>
</tr>
</thead>
<tbody>
<tr>
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Motivation: Bias/Error versus Speed

Importance of Computational Efficiency:
Garcia-Menendez (in prep) recommends at least 15 years (depending on region) to get signal out of variability.

Will be Different Depending on Region (Global, US, NEUS, etc.)

Years Simulated for Same Computational Cost as MOZART

Core Hours Per Simulated Year
Comparing Meteorologies


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O3 ppb

PM2.5 ug/kg
## Comparing Meteorologies

### Relative Difference:

<table>
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<tr>
<td>JJA Surface O3</td>
<td>-30%</td>
</tr>
<tr>
<td>JJA Surface PM2.5</td>
<td>+60%</td>
</tr>
<tr>
<td></td>
<td>+70%</td>
</tr>
<tr>
<td></td>
<td>+10%</td>
</tr>
<tr>
<td></td>
<td>+150%</td>
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</table>

### Widget:

- **JJA Surface O3**:
  - +50%
  - -50%

- **JJA Surface PM2.5**:
  - 1:1
  - -50%
  - +50%

---

### Maps:

- **O3**
  - 12 Nov 2005 04:00
  - +70%
  - +100%
  - +5,000+%

- **PM2.5**
  - 13 Jul 2005 12:00
  - +100%
  - +400%
  - +5,000+%
Comparing Mechanisms

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O₃ ppb

PM2.5 ug/kg
Reduced Hydrocarbon Mechanism (Houweling et al., 1998)

Simplified treatment of hydrocarbons
- Different Lumping:
  - Alkanes – Paraffins
  - Alkenes - Olefins

Additionally:
- Removed Halogen Species (as Stratosphere is Specified), which results in 40%+ faster simulations with only small differences at the surface compared to “full” Reduced Hydrocarbon Mechanism
For Ozone:
Superfast Mechanism
(Cameron-Smith et al., 2006, Lamarque et al. 2013, others)

For PM2.5:
BAM-Only

Comparing Mechanisms

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SFM or BAM
MOZ

Relative Difference

For Ozone:
Superfast Mechanism
(Cameron-Smith et al., 2006, Lamarque et al. 2013, others)

For PM2.5:
BAM-Only
Computational Advantages

United States Grid Cells

Core Hours Per Simulated Year

- CAM-Chem
- GEOS5
- Reduced HC5s
- RHCM

- CAM-Chem
- IGSM-CAM
- MOZART
- IC_Met

O3 ppb

30 ppb

50 ppb

40 ppb

46.2±2.8

11 ppb

35.5±2.5

50.3±2.8

33%

4 ppb

4 ppb

4 ppb

60%

33%
Quantifying RHCM Acceptability

Difference in Means Test
To determine is RHCM is Different from MOZART (taken from Wilks, 2006)

\[
Z = \frac{\bar{x}_{MOZ} - \bar{x}_{RHCM}}{\sqrt{\frac{S_{MOZ}^2}{n_{MOZ}} + \frac{S_{RHCM}^2}{n_{RHCM}}}}
\]

H\text{\textsubscript{o}}: underlying means are equal
H\text{\textsubscript{A}}: not equal

As surface time series data for O\textsubscript{3} and PM\textsubscript{2.5} are highly autocorrelated (\(\rho_1 \sim 0.7 - 0.9\))
I use the effective sample size (n\textquotesingle) instead of the full sample size (n = 368)

\[
n' = n \frac{1 - \rho_1}{1 + \rho_1}
\]
Using $n'$

p-values for: (Ho: no difference in mean between MOZ and RHCM)

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Each grid cell

5 cells in every direction

10 cells in every direction
How do they all compare?

Percent Difference from MOZART Ozone Simulations

*preliminary
First Pass: using GEOS-Chem’s emissions in CAM-Chem
Near Future: GEOS-Chem simulations, direct comparison

- Relative Difference: \[
\frac{\text{CAM-Chem with GEOS-Chem Emissions}}{\text{CAM-Chem with CAM-Chem Emissions}}
\]
Next Steps

• GEOS-Chem Simulations → Structural Uncertainties
  • standard full tropospheric chemistry
    • GEOS5 and IGSM-CAM meteorology
  • 4x5 degree (maybe T31?) simulations
    • (CAM-Chem and GEOS-Chem)
    • Aiming for maximum efficiency/ensemble sizes

• Comparison to Observations

• Population-Weighted Statistics
  • for Human Health Impacts (e.g. via BenMAP)

MOZART

population weighted MOZART
Thanks!

• MIT:
  • Noelle Selin, Ron Prinn, Erwan Monier, Fernando Garcia-Menendez + many others

• NCAR:
  • Louisa Emmons, Simone Tilmes, Gabi Pfister + others

• LLNL:
  • Philip Cameron-Smith
Extra Slides
More Details About the “Reduced” RHCM

All these Plots:
RHCM Mechanism/MOZART

Surface Values, Average JJA, Daily, 2004 - 2007

Difference Between Regular RHCM and Reduced RHCM:

DATA MINIMUM= 0.9999970 MAXIMUM= 1.0000005
• Not surprising, as we’ve removed much of the halogen chemistry, which strongly impacts ozone chemistry over Antarctica
• Everywhere else, there does not seem to be a significant difference in O3 chemistry

If I exclude the southern polar region:
**O₃**

**MOZART**

**NOTE:**
- same color scales

**Absolute Values**

**Relative Difference from MOZART**

**NOTE:**
- different color scales
NOTE: same color scales

Absolute Values

Relative Difference from MOZART

NOTE: different color scales

south of 50 lat

north of 50 lat

Reduced Hydrocarbon

MOZART

NO
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10 cells in every direction

n = 368

n' < 250

n' < 100

n' < 40
use $n=368$

p-values for: (H0: no difference in mean between MOZ and RHCM)

each grid cell

5 cells in every direction

10 cells in every direction

relative difference (RHCM/MOZ)