DYNAMO: DYnamic Inputs of Natural Conditions for Air Quality MODELS

AQAST Tiger Team
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Key Additional Participants in DYNAMO

Air Quality Management partners:
• EPA: Jesse Bash, Pat Dolwick, Chris Misenis
  – 2011 CMAQ CONUS simulation
• Texas Commission on Environmental Quality: Mark Estes
• California Air Resources Board: Jeremy Avise

Students: Ben Lash (Rice), Erin Chavez Figueroa (Rice), Quazi Rasool (Rice), and Lulu Shen (Harvard)

Postdoc: Dr. Rui Zhang (Rice)
DYNAMO Objectives

- **Stratospheric ozone**: Satellite-based daily varying columns, to replace weekly averages
  - GEOS-Chem simulations showed small impacts in summer, when stratospheric $O_3$ is less variable

- **Clouds & Radiation**: GOES-based clouds for photolysis rates and photosynthetically active radiation (PAR)
  - Presentation by Arastoo Pour Biazar

- **Interannual variability in biogenic VOC**
  - Influence of drought, temperature, and PAR

- **Soil NO**: Implement & extend BDSNP scheme
  - Impacts on $NO_2$ columns, ozone, and PM
WRF and MEGAN runs for 2005 and 2007 to test influence of drought and T on isoprene
Year 2005 and 2007 MEGAN simulations to test sensitivities to meteorological and LAI variability

- **Compute partial sensitivities**
  - Leaf Area Index
    - With constant T and PAR
  - Radiation (PAR)
    - With constant LAI
  - Temperature
    - With constant LAI

\[
\frac{\Delta ISOP}{\Delta LAI} = \left( \frac{ISOP,2007 - ISOP,2005}{LAI,2007 - LAI,2005} \right)
\]

\[
\frac{\Delta ISOP}{\Delta PAR} = \left( \frac{ISOP,UMDPAR,2005 - ISOP,WRFPAR,2005}{PAR,UMD,2005 - PAR,WRF,2005} \right)
\]

\[
\frac{\Delta ISOP}{\Delta T} = \left( \frac{ISOP,2007 - ISOP,2005}{T,2007 - T,2005} \right)
\]

- **Evaluations by biome over four regions**
Sensitivities of isoprene emissions to LAI, PAR, and temperature

**S CA July**

**NE US July**

**E TX July**

**SE US July**
2005→2007 change in MEGAN isoprene (blue shows change due to $\Delta$PAR)

$$
\frac{\Delta ISOP}{\Delta PAR} = \left( \frac{ISOP, UMD, PAR, 2005 - ISOP, WRF, PAR, 2005}{PAR, UMD, 2005 - PAR, WRF, 2005} \right) \times \left( \frac{PAR, WRF, 2007 - PAR, WRF, 2005}{PAR, WRF, 2005} \right)
$$
Fractional reduction in MEGAN BVOC emissions due to using Pinker satellite PAR vs. WRF

July 2007 simulation

Isoprene

Monoterpenes

Sesquiterpenes
New Soil NO Emissions Scheme in CMAQ

• Berkeley Dalhousie Soil NO Parameterization (BDSNP)
  – Introduced by Hudman et al. 2012; In GEOS-Chem
• Ben Lash (Rice) implemented in CMAQ (inline biogenics)
  – Provided to EPA (J. Bash) for upcoming CMAQ release
  – Also shared with UMD and other interested parties
• Base-level emissions factors for each land cover category based on Steinkamp and Lawrence 2011
• Fertilizer and N deposition add N to soil reservoir
• Meteorology influences emissions
  – Soil moisture and T from land surface model, instead of rainfall and air T
  – Pulse of emissions when rain follows dry period
Soil NO emissions components in BDSNP (CMAQ for CONUS 2005)

- Nationally, biome factor is biggest contributor
- Fertilizer >50% in Midwest, San Joaquin Valley
- Deposition >50% in southern California, Atlanta
Soil NO emissions in CMAQ simulation for CONUS 2005

ngN/m²/s monthly averages

Month

CMAQ
BDSNP

CMAQ
Yienger & Levy
BDSNP >> Y&L for Soil NO Emissions
(Change in NO emissions per cell for Aug. 2005)

BDSNP ~ 2x Y&L soil NO in summer, but with very different spatial patterns and responses to meteorology -- Can’t just scale Y&L.
Schemes have very different assumed responses of soil NO to temperature and moisture

- Hudman et al. 2012
Fractional change in NO$_2$ columns due to BDSNP
CMAQ_BDSNP overpredicts OMI NO$_2$ columns, but BDSNP not responsible in California and Northeast.

Monthly averages (*10$^{15}$ molecules/cm$^2$) in OMI v. 2.1 (from L. Lamsal) and CMAQ_BDSNP for 2005.

<table>
<thead>
<tr>
<th>Month</th>
<th>April</th>
<th>May</th>
<th>June</th>
<th>July</th>
<th>August</th>
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<tr>
<td><strong>Satellite</strong></td>
<td>1.50</td>
<td>1.23</td>
<td>1.22</td>
<td>1.04</td>
<td>1.06</td>
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<tr>
<td><strong>CMAQ-BDSNP</strong></td>
<td>1.71</td>
<td>1.50</td>
<td>1.42</td>
<td>1.43</td>
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</tr>
</tbody>
</table>
Changes in OH and $O_3$, BDSNP – YL
(August 2005 avg.)

August 2005 CMAQ simulation
Impact of BDSNP on $O_3$ sensitivity to 10% anthropogenic NO$_x$ reduction

On a fractional basis, higher soil NO reduces sensitivity to anthropogenic NO$_x$ by 10-40% over much of Midwest and Northwest.
Rain induced pulsing event on July 3, 2011 in CMAQ-BDSNP

Note: BDSNP assumes a pulsing event occurs when rain follows a dry period, activating soil microbes and causing enhanced soil NO emissions.
BDSNP – YL for NO emissions, NO$_x$, ozone, and OH: July 3, 2011
BDSNP can increase PM$_{2.5}$ by $>1$ ug/m$^3$, largely due to particulate water (7/3/2011)
Fractional increase in NO$_2$ column due to BDSNP

![Map showing NO$_2$ Column fraction (BDSNP–YL95)/(YL95) on July 3, 2011 at 00:00:00 UTC. The map illustrates the variation across the United States with values ranging from -0.2 to 1.3. The minimum value is at (103, 129) with a value of -0.1, and the maximum value is at (177, 140) with a value of 1.2.](image-url)
Is BDSNP soil NO still too low?

- Vinken (ACP 2014) estimates 12.9 ± 3.9 TgN/yr from OMI, vs 9.6 in BDSNP
  - Out of 51 TgN total NO\textsubscript{x} globally
  - Used DOMINO v. 2.0 for OMI NO\textsubscript{2}
Is BDSNP too high over N. America?

- Vinken OMI-based estimate was lower than BDSNP over central US in 2005
- Hudman assumes 1.5% of fertilizer N is emitted as NO, vs. 0.5-1% in most studies
- N. American biome emission factors from Steinkamp are lower than global used by BDSNP

Vinken et al., ACP 2014
Intended Extensions of BDSNP Soil NO

• EPIC dynamic fertilizer to replace Potter et al. 2010
• Test N. America biome factors and lower fertilizer factor
• More evaluations vs. ambient & satellite NO₂
  – Are the pulsing events “real” and observed by OMI??
• Offline version of BDSNP for direct creation of soil NO emissions using WRF or other meteorology data
  – Requires assumptions about N-deposition
• Add soil emissions of HONO (Su et al. 2011)
• Test sensitivities to agricultural practices (e.g., fertilizer application, biochar, etc.)
• Ultimate goal: More mechanistic model to simulate all soil N emissions (NO, NH₃, HONO, N₂O, etc.)
Extra Slides
Impact of UAH satellite PAR on emissions
Sept. 2013 simulation

Base Emissions from MEGAN

Satellite (UAH) minus WRF

Isoprene

(a-1) Average daily mean Isoprene emission rate (mol/s) using modeled PAR (WRF)

(a-2) Relative difference of MEGAN Isoprene emission rate using PAR between satellite retrieval (UAH) and model (WRF)

Monoterpines

(b-1) Average daily mean Monoterpene emission rate (mol/s) using modeled PAR (WRF)

(b-2) Relative difference of MEGAN Monoterpene emission rate using PAR between satellite retrieval (UAH) and model (WRF)
Isoprene Change due to PAR 2005 to 2007

\[
\frac{\Delta ISOP}{\Delta PAR} = \left( \frac{ISOP, UMD, PAR, 2005 - ISOP, WRF, PAR, 2005}{PAR, UMD, 2005 - PAR, WRF, 2005} \right) \times \left( \frac{PAR, WRF, 2007 - PAR, WRF, 2005}{PAR, WRF, 2005} \right)
\]
Motivation: Pinker (UMD) satellite-based insolation better matched observations than WRF, but no longer available.
Change in ozone concentrations due to BDSNP
ASO4 (BDSNP–YL95)

July 3, 2011 00:00:00 UTC
Min (161, 142) = -0.039, Max (275, 120) = 0.115
OH(BDSNP–YL95)

July 3, 2011 00:00:00 UTC

Min (158, 128) = -3.026E-8, Max (169, 125) = 8.203E-8
Changes in OH and O$_3$, BDSNP – YL
(August 2005 avg.)

August AVG OH BDSNP - YL

August AVG O3 BDSNP - YL

August 2005 CMAQ simulation