Evaluation of Model Simulated Ozone and its Precursors Using the Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICA) during the Michigan-Ontario Ozone Source Experiment (MOOSE)

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Ozone levels continue to **exceed NAAQS standards** in SEMI.

Many **factors** are **associated with** O$_3$ **exceedance** (e.g., precursor emissions, long-range transport, meteorology, land-lake interactions).

More detailed and innovative measurements and modeling studies are necessary for understanding O$_3$ production and loss in SEMI.
Black residents of Detroit brace themselves for rougher air quality conditions

Detroit's air quality is among the worst in the world because of the Canadian wildfires, exposing an already-vulnerable population to more health risks.
A. Investigate the sensitivity of model simulated O\textsubscript{3} and its precursors to model horizontal grid resolutions in MUSICAv0.
   1. Create ~7 km (1/16°) grid over Michigan.
   2. Implement and evaluate new grid.

B. Quantify the drivers of O\textsubscript{3} nonattainment in Southeast Michigan using optimal MUSICAv0 model grid.
   1. Implement diurnal cycle for NO emissions
   2. Identify and quantify physical and chemical drivers of O\textsubscript{3} production and loss in SEMI through emission sensitivity experiments.
• Led by Michigan Department of Environment, Great Lakes, and Energy (EGLE), with participants from universities, federal agencies, and Environment Climate Change Canada.

• Seeks to define potential attainment strategies in SEMI region and better understand what contributes to excess O$_3$.

• **Phase I: May 24 – June 30, 2021**

• **Phase II: June 6-28, 2022**

• **Varied, High-Resolution Measurements**
  • Aircraft (NASA G-III), Mobile Lab (Aerodyne), Stationary

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**MICHIGAN-ONTARIO OZONE SOURCE EXPERIMENT (MOOSE)**

From left to right: Noribeth Mariscal, Erin Browne, Jiajue Chai, Debatosh Partha, Yaoxian Huang, Heejeong Kim
**Multi-Scale Infrastructure for Chemistry & Aerosols, Version 0**

- Configuration of CESM/CAM-Chem
- Uses Spectral Element (SE) Dynamical Core
- Regional Refinement (RR)
- Described in Pfister et al (2020)
- Default Resolution:
  - ~14 km Latitude x ~14 km Longitude (1/8°) over CONUS
  - 32 Vertical Layers (~40 km Model Top)

**Model Configuration:**
- April-August 2021
- Initial Conditions based on SE 1° CAM-Chem Run
- NASA MERRA-2 (Resolution: 0.625° x 0.5° every 3 hours)
- MOZART-TS2
- CAMS-GLOB-ANTv5.1, CAMS-GLOB-AIRv2.1, QFED, MEGANv2.1
Regional Refinement over Michigan

- Community Mesh Generation Toolkit
- ne30x8 CONUS → ne30x16 MICH
- ~7 km Latitude x ~7 km Longitude over Michigan
- Smooth transition (halo) between resolutions to mitigate potential errors
- Time Step: 3.75 mins
COMPARISON WITH SEMI STATIONARY SITE

Allen Park [062021]

- O₃ [ppb]: MB: -6.9
- O₃ [ppb]: MB: -7.4
- NOₓ [ppb]: MB: 13.7
- NOₓ [ppb]: MB: 13.8
- T [K]: MB: 2.3
- T [K]: MB: -0.2

Urban-Suburban Mix

Detroit – E 7 Mile [062021]

- O₃ [ppb]: MB: -1.1
- O₃ [ppb]: MB: -0.1
- NOₓ [ppb]: MB: 4.1
- NOₓ [ppb]: MB: 1.7
- T [K]: MB: 2.4
- T [K]: MB: -0.2

\[ MB = \bar{M} - \bar{O} \]
COMPARISON WITH AML

MUSICAv0 Ozone ($O_3$) Compared to MOOSE Aerodyne Mobile Lab Observations

$O_3$ [ppb]

MUSICAv0 Nitrogen Oxide ($NO_x$) Compared to MOOSE Aerodyne Mobile Lab Observations

$NO_x$ [ppb]

MUSICAv0 Temperature Compared to MOOSE Aerodyne Mobile Lab Observations

$T$ [deg-C]

$MB = \bar{M} - \bar{O}$
COMPARISON WITH AML

MUSICAv0 Ozone Compared to MOOSE Aerodyne Mobile Lab Observations

MUSICAv0 Ozone ($O_3$) Compared to MOOSE Aerodyne Mobile Lab Observations

MUSICAv0 Nitrogen Oxide ($NO_x$) Compared to MOOSE Aerodyne Mobile Lab Observations

MUSICAv0 Temp

MB: -2.9 | MB: -1.3

MB: -6.2 | MB: -1.8

MB: 0.8 | MB: -0.4

MB: -0.2 | MB: -0.7

MB: 1.3 | MB: -0.2

Model is not capturing some daily trends!

$MB = \bar{M} - \bar{O}$
IMPLEMENTATION OF DIURNAL CYCLE FOR NO

CAMSv5.1 NO Emissions in e^{12} molecules cm^{-2} s^{-1}

<table>
<thead>
<tr>
<th></th>
<th>MICH [kt]</th>
<th>SEMI [kt]</th>
<th>SEMI/MICH</th>
</tr>
</thead>
<tbody>
<tr>
<td>AGS</td>
<td>0.46</td>
<td>0.04</td>
<td>9.0%</td>
</tr>
<tr>
<td>AWB</td>
<td>0.10</td>
<td>0.01</td>
<td>10.8%</td>
</tr>
<tr>
<td>ENE</td>
<td>9.44</td>
<td>2.86</td>
<td>30.3%</td>
</tr>
<tr>
<td>RES</td>
<td>1.03</td>
<td>0.48</td>
<td>47.1%</td>
</tr>
<tr>
<td>TNR</td>
<td>1.99</td>
<td>0.36</td>
<td>18.1%</td>
</tr>
<tr>
<td>TRO</td>
<td>15.13</td>
<td>3.50</td>
<td>23.2%</td>
</tr>
</tbody>
</table>

- Important in evaluating model uncertainties
- Diurnal variations for anthropogenic emissions are NOT considered in CESM2.
- Heavily influences regions with many anthropogenic sources.
ON-GOING & FUTURE WORK

- Complete MUSICAv0 runs with diurnal cycle for NO emissions for the ne30x8 CONUS and ne30x16 Michigan grids
  - Regrid emission files to include sectors
  - Add in diurnal information files
  - Evaluate runs with MOOSE Phase I campaign datasets

- Run suite of sensitivity experiments to quantify contribution of emission from various sectors and long-range transport on O$_3$ in SEMI.

- Combine MUSICAv0 with an exposure model to study impacts of O$_3$ nonattainment on human health in SEMI.

<table>
<thead>
<tr>
<th>Case</th>
<th>Grid Name</th>
<th>Resolution (km)</th>
<th>Setup</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>ne30x16</td>
<td>~7</td>
<td>Control</td>
</tr>
<tr>
<td>2</td>
<td>ne30x16</td>
<td>~7</td>
<td>TRO*-OFF</td>
</tr>
<tr>
<td>3</td>
<td>ne30x16</td>
<td>~7</td>
<td>ENE*-OFF</td>
</tr>
<tr>
<td>4</td>
<td>ne30x16</td>
<td>~7</td>
<td>OTH*-OFF</td>
</tr>
<tr>
<td>5</td>
<td>ne30x16</td>
<td>~7</td>
<td>ALL*-OFF</td>
</tr>
</tbody>
</table>
ACKNOWLEDGEMENTS

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I would like to acknowledge the high-performance computing support from Cheyenne (DOI: https://doi.org/10.5065/D6RX99HX) provided by NCAR’s Computational and Information Systems Laboratory, sponsored by NSF, and the Grid High Performance Computing (HPC) support from Wayne State University.

I’d like to thank:

o My collaborators: Yaoxian Huang (WSU), Louisa K. Emmons (NCAR), Duseong S. Jo (NCAR), Ying Xiong (WSU), and Jiajue Chai (SUNY)

o Tara Yacovitch, Brian Lerner, and Francesca Majluf of Aerodyne Research, Inc. and the rest of the MOOSE Science Teams for the campaign datasets used in this study.
thank you!

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questions?
backup slides.
• April-August 2021
  • April used as a spin up
• Initial conditions based on SE 1° CAM-Chem run
• NASA MERRA-2 (Resolution: 0.625° x 0.5° every 3 hours)
  • Meteorological nudging not applied to Michigan [41°N, 272.5°W]
• MOZART-TS2
  • Comprehensive representation of tropospheric and stratospheric chemistry with updated gas-phase chemistry for isoprene and terpene species
• MAM4: Spatial distribution of aerosols
• VBS-SOA: secondary organic aerosols separation
• Emissions
  • CAMS-GLOB-ANTv5.1 (Anthropogenic)
  • CAMS-GLOB-AIRv2.1 (Aircraft)
  • QFED (Biomass Burning)
  • MEGANv2.1 (Biogenic)
Anthropogenic and biomass burning emissions are generated offline and regridded to corresponding resolution.

- **Copernicus Atmosphere Monitoring Service Version 5.1 (CAMS-GLOB-ANTv5.1)**
  - Global anthropogenic emissions based on monthly emissions from EDGARv5 and CEDSv2
  - Resolution: 0.1° x 0.1°
  - Sectors: ENE, RCO, TRO, TNR, FEF, IND, SLV, AGR, MMA, SHP, SWD

- **CAMS-GLOB-AIRv2.1**
  - Aircraft emissions
  - Resolution: 0.5° x 0.5°
### STATIONARY MEASUREMENTS

<table>
<thead>
<tr>
<th>Site Name</th>
<th>Coordinates</th>
<th>Description¹</th>
<th>Types of Measurements²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Allen Park</td>
<td>42.22°N, 276.8°W</td>
<td>Suburban</td>
<td>O₃, NOₓ, T, WS, WD</td>
</tr>
<tr>
<td>E 7 Mile</td>
<td>42.43°N, 277.0°W</td>
<td>Urban Suburban Mix</td>
<td>O₃, NO₂, T, WS, WD</td>
</tr>
<tr>
<td>New Haven</td>
<td>42.73°N, 277.21°W</td>
<td>Coastal</td>
<td>O₃, T, WS, WD</td>
</tr>
<tr>
<td>Oak Park</td>
<td>42.47°N, 276.82°W</td>
<td>Suburban</td>
<td>O₃, T, WS, WD</td>
</tr>
<tr>
<td>Port Huron</td>
<td>42.95°N, 277.55°W</td>
<td>Downwind</td>
<td>O₃, T, WS, WD</td>
</tr>
<tr>
<td>Trinity St Marks³</td>
<td>42.3°N, 276.87°W</td>
<td>Urban</td>
<td>O₃, CO, NO, NO₂, WS, WD</td>
</tr>
<tr>
<td>Ypsilanti</td>
<td>42.24°N, 276.4°W</td>
<td>Suburban</td>
<td>O₃, T, WS, WD</td>
</tr>
</tbody>
</table>

¹Description of where the site is located.
²O₃ = Ozone; NO = Nitric Oxide; NO₂ = Nitrogen Dioxide; NOₓ = sum of NO₂ and all other reactive nitrogen; T = Temperature; WD = Wind Direction; WS = Wind Speed; CO = Carbon Monoxide.
³The Trinity St Marks site contains measurements of CO, NO₂, WS, and WD collected from MASN, as well as measurements of O₃, NO, and NO₂ from Chai et al., 2023, In Preparation.
COMPARISON WITH SEMI STATIONARY SITE

\[ MB = \bar{M} - \bar{O} \]
COMPARISON WITH SEMI STATIONARY SITE

Urban

Urban-Suburban Mix

Urban

Urban
Run suite of sensitivity experiments to **quantify** contribution of emission from various sectors and long-range transport on $O_3$ in SEMI.

Help identify the impact on $O_3$ from different emission sectors, in order to better determine how to reach $O_3$ attainment in SEMI.

**Table 1:** Anthropogenic emission totals for May and June 2021 based on the CAMS-GLOB-ANTv5.1 emission inventory for Michigan and Southeast Michigan.

<table>
<thead>
<tr>
<th>Species</th>
<th>Molecular Weight [g/mol]</th>
<th>Michigan [Gg]</th>
<th>Southeast Michigan [Gg]</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>28</td>
<td>201.6</td>
<td>59</td>
</tr>
<tr>
<td>NO</td>
<td>30</td>
<td>34.3</td>
<td>10</td>
</tr>
<tr>
<td>SO$_2$</td>
<td>64</td>
<td>19.4</td>
<td>6.5</td>
</tr>
<tr>
<td>C$_2$H$_6$</td>
<td>30</td>
<td>1.2</td>
<td>0.3</td>
</tr>
<tr>
<td>C$_3$H$_8$</td>
<td>44</td>
<td>1.1</td>
<td>0.5</td>
</tr>
<tr>
<td>HCHO</td>
<td>30</td>
<td>0.7</td>
<td>0.2</td>
</tr>
<tr>
<td>BENZENE</td>
<td>78</td>
<td>0.8</td>
<td>0.3</td>
</tr>
<tr>
<td>TOLUENE</td>
<td>92</td>
<td>3.3</td>
<td>1.6</td>
</tr>
<tr>
<td>XYLENES</td>
<td>106</td>
<td>6.1</td>
<td>3</td>
</tr>
<tr>
<td>BIGALK$^*$</td>
<td>72</td>
<td>9.8</td>
<td>3.3</td>
</tr>
<tr>
<td>BIGENE$^*$</td>
<td>56</td>
<td>1.1</td>
<td>0.4</td>
</tr>
</tbody>
</table>

$^*$BIGALK represents lumped alkanes of C>3 (i.e., butanes, C$_4$H$_{10}$, and larger); BIGENE represents lumped alkenes of C>3 (i.e., butenes and larger) (Emmons et al., 2020).
CAM Sv5.1 NO Emissions in $e^{12}$ molecules cm$^{-2}$ s$^{-1}$