A Better Representation of VOC chemistry from VCP and Cooking emissions in WRF-Chem

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Development of RACM2B_VCP chemical mechanisms

**RACM2_Berkeley2.0:**
RACM2 with more complex representation of organic nitrates especially for biogenics VOCs (Goliff et al., 2013; Browne et al., 2014; Zare et al., 2018)

- **Add VCP VOC chemistry:**
  isopropanol, propylene glycol, and glycerol (Coggon et al., 2021)

- **Photolysis:**
  Incorporate new photolysis scheme (new TUV, opt=4)
  Add the boundary layer clouds and ingest the full 3D GFS O3

- **Aerosol scheme:**
  Couple the updated SOA scheme in RACM_ESRL_VCP (Ahmadov et al., 2012)

- **Aerosol uptake:**
  added aerosol uptake of inorganic species and revised aerosol uptake of organic nitrates

- **Add new emission tracers:**
  Added VCP and cooking tracers to the chemistry to fully evaluate the emissions
### Representation of VCP and Cooking emission tracers in WRF-Chem

**Gkatzelis et al., 2021**

<table>
<thead>
<tr>
<th>Species</th>
<th>D4-Siloxane, D5-Siloxane, PCBTF, PDCBZ</th>
<th>Nonanal, Octanal, CALD (saturated aldehydes from cooking), CUALD (unsaturated aldehydes from cooking)</th>
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<tbody>
<tr>
<td>Reactions</td>
<td>OH (D4-siloxane: 1.3e-12, D5-siloxane, 2.1e-12, PCBTF: 2.4e-13, PDCBZ: 3.2e-13)</td>
<td>OH, NO₃, photolysis O₃ reactions with CALD and CUALD Atkinson and Arey 2003; Jenkin et al., 2018</td>
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<tr>
<td>Emissions</td>
<td>Coggon et al., 2021 + re-speciation</td>
<td>Coggon et al., in prep, based on obs from SUNVEX</td>
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</tbody>
</table>
Evaluation of WRF-Chem simulated VOC chemistry using RECAP and SUNVEX measurements

June 2021 NPS Twin Otter airborne measurements (RECAP)

August 2021 CSL Mobile Laboratory (SUNVEX)

We categorize the flight/mobile tracks into four regions: **Downtown LA, San Bernadino Valley, Santa Anna Valley, Coastal LA.**
Evaluation of WRF-Chem simulated VCP tracers

- WRF-Chem reproduces the observed range of D5-siloxane and PCBTF from both RECAP and SUNVEX measurements.
Evaluation of WRF-Chem simulated cooking emission tracers

RECAP
• Nonanal (NALD) and octanal (OALD) is added to the WRF-Chem as cooking emission tracers.
• The good agreement of nonanal and octanal between model and observations validate the cooking emissions in the current emission inventories.

SUNVEX
Evaluation of VOC reactivity in WRF-Chem by comparing against RECAP

Aromatics: benzene, toluene, xylene
VCP tracer: D5SILX, D4SILX, PCBTF, PDCBZ
Cooking tracer: CALD, CUALD, NALD, OALD
Evaluation of VOC reactivity in WRF-Chem by comparing against RECAP

64% of VOC reactivity attributes to species that are measured and calibrated during RECAP.

WRF-chem is 32% lower in calibrated VOC reactivity compared to RECAP.
Evaluation of VOC reactivity in WRF-Chem by comparing against RECAP

Ethanol and monoterpenes are two dominant VOCs contributing to the low bias in VOC reactivity.
Evaluation of WRF-Chem simulated O₃ using AQS surface network

Observed MDA8 O₃ map from AQS

![Map showing observed MDA8 O₃ levels across LA with color-coded areas for different scales.]

- Micro: 0m – 100m;
- Middle: 100m – 500 m;
- Neighbor: 500m – 4km;
- Urban: 4km – 50 km

WRF-Chem reproduces AQS observed surface O₃ over LA except two sites representing microscales.
Investigate the impact of VCP and cooking emissions on VOC reactivity and O$_3$

Besides the model run with full VOC emissions (#0), we conducted two sensitivity test runs:
#1 Emissions without cooking emissions;
#2 Emission without cooking + VCP emissions

We define
Cooking emission impacts: simulation #0 – simulation #1
VCP emission impacts: simulation #1 – simulation #2
Investigate the impact of VCP and cooking emissions on total VOC reactivity

VOC reactivity is sampled along RECAP flight tracks. Cooking and VCP emission contribute to 12% and 22% of the VOC reactivity, respectively.
Investigate the impact of VCP and cooking emissions on O$_3$

Changes in MDA8 O$_3$ due to cooking emission

Changes in MDA8 O$_3$ due to VCP emission

surface MDA8 O$_3$ from WRF-Chem
Conclusion

- VOC chemistry and ozone are well presented in WRF-Chem using a new developed RACM2_BERK_VCP_SILX_NALD chemical mechanism in this study.
- WRF-Chem still has a low bias in VOC reactivity, predominantly due to the underestimate in ethanol and monoterpene.
- We conducted sensitivity tests to investigate the impacts of cooking and VCP emissions on VOC reactivity and MDA8 ozone over LA.

Future work

- Finish WRF-Chem model runs at finer 4 km horizontal resolution.
- Expand sensitivity tests to biogenic and anthropogenic VOC emissions.
- Tackle the issue of low bias in monoterpene and ethanol

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