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Modeling the Formation of SOA from Volatile Chemical Products in Los Angeles

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Volatile chemical product (VCP) emissions

- VCPs are commonly-used consumer and industrial items
 - personal care products
 - cleaning products
 - paints & coatings
 - printing inks
 - adhesives & sealants
 - pesticides
- Increasingly important source of anthropogenic emissions¹
- The VCPy framework allows for estimation of VCP emissions²



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SOA yields fall in 5 categories



Data

- Statistical Oxidation Model (Cappa & Wilson, 2012; McDonald et al., 2018)
- Laboratory studies (Presto et al., 2010; Tkacik et al., 2012; Ng et al., 2007; Hildebrandt et al., 2009; Janecheck et al., 2019; Wu and Johnson 2017; Li and Cocker 2018; Charan et al., 2020)





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New VCP chemical mechanism development







VCPy emissions speciation

- Individual species assigned to model surrogates using updated speciation mapping (SAPRC07TIC_AE7_VCP)
- Outer ring: Los Angeles County 2010 emissions speciation assignments
- Inner ring:
 - Hatched: emissions originally assigned to model surrogates that do not participate in model chemistry (IVOC, NVOL, and NROG)
 - Solid: other surrogate assignments
- 44% of VCP emissions are SOA precursors









Community Multiscale Air Quality (CMAQ) model simulations

- California 4 km grid, May 15 June 15, 2010
- CMAQ version 5.3.2beta
- WRF version 3.8.1 meteorology
- NEI 2011 emissions inventory + VCPy version 1.0 emissions^{1,2}
- SAPRC07TIC + aero7i + VCP chemical mechanism³ + mobile IVOC treatment⁴
- Observations provided during the CalNex campaign⁵

¹Seltzer et al., ACP, 2017
²Seltzer et al., in review
³Pennington et al., ACPD, 2021
⁴Lu et al., ACP, 2020
⁵Ryerson et al., JGR, 2013





form negligible SOA.

VCPs double SOA formation in Pasadena



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VCPs improve model representation of other criteria pollutants

- Ratio of modeled to observed values improved
 - SOA: 0.23 → 0.43

• Formaldehyde: $0.58 \rightarrow 0.75$

• Ozone: 0.72 → 0.95







SOA & formaldehyde bias vs. temperature

- Formaldehyde bias and SOA bias demonstrate similar relationship to temperature
- Investigations of formaldehyde could provide insight into VOC chemistry leading to the formation of SOA from VCPs.
- POA and CO do not follow the same trend





- VCPs are an important source of anthropogenic emissions and precursors to SOA formation.
- VCPs contribute 1.66 μg m⁻³ of average total noontime SOA up to half of anthropogenic SOA in Los Angeles.
- Formaldehyde and SOA show similar relationships to temperature and bias signatures indicating common sources and/or chemistry.

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Modeling SOA formation in Los Angeles during the COVID-19 pandemic, springsummer 2020

- Southern California experienced a large reduction in mobile emissions during the COVID-19 pandemic alongside periods of extreme heat and high rainfall
- These nonlinear interactions led to an uneven impact on criteria pollutants throughout the Los Angeles Basin¹

Average percent traffic level reduction March 19-June 30 compared to January-February¹









Los Angeles 2020: Conclusion & Goals

Simulation Case(s)	Model Configuration	Goal
base	Base case described in previous slides.	Replicate observations and understand the source apportionment, chemistry, and speciation of SOA and other criteria pollutants in Los Angeles.
0x_VCP, 0x_onroad, 0x_bio	Zero out VCP, onroad, or biogenic emissions.	Quantify the effect of VCP, onroad, biogenic, and other (via subtraction) emissions on SOA.
preCOVID_onroad	Scale onroad emissions to 2019 pre-COVID VMT data.	Predict the air quality impact of COVID-19 emissions, maintaining 2020 meteorology.
scaled_VCP	Scale VCP emissions (≶1) using VCPy uncertainty bounds.	Investigate the impact of past/future scenarios of VCP use and composition.
base_ISAM	Turn on CMAQ ISAM.	Understand the contribution of different factors (e.g. boundary conditions, each emission source) on O_3 and NO_x concentrations.





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