EPA United States Environmental Protection Agency

A New Model to Represent SOA Formation from Volatile Chemical Products

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Volatile chemical products (VCPs) are an important source of anthropogenic emissions

Personal care products

Cleaning products

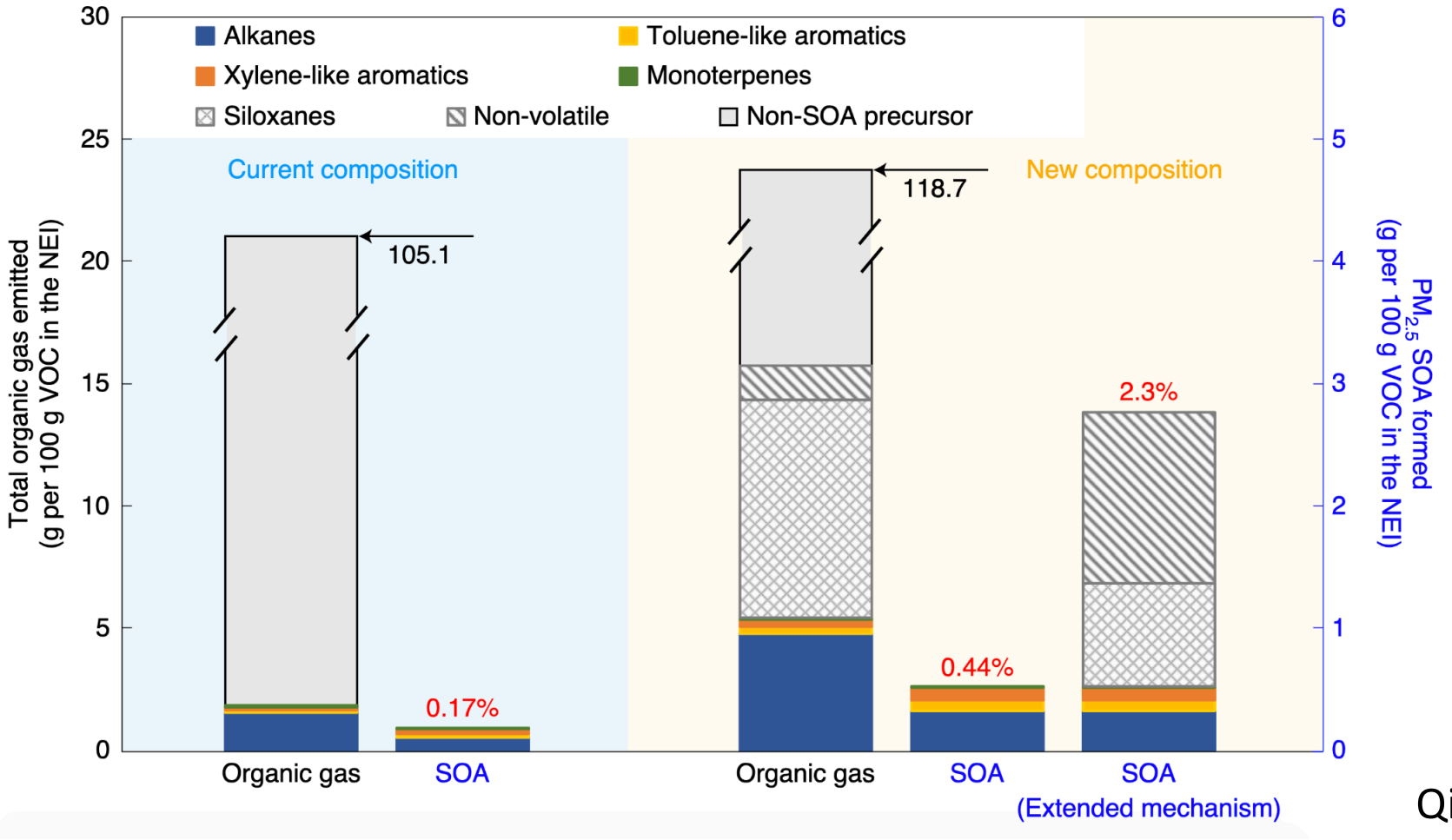
Paints & Coatings

Pesticides

Printing inks

Adhesives & Sealants

Volatile chemical products (VCPs) make secondary organic aerosol (SOA)



Qin et al., 2020

Objectives

1. VCP emissions
2. VCP species properties
3. Model development
4. CMAQ simulation results
5. Conclusions

Personal care products

Cleaning products

Paints & Coatings

Pesticides

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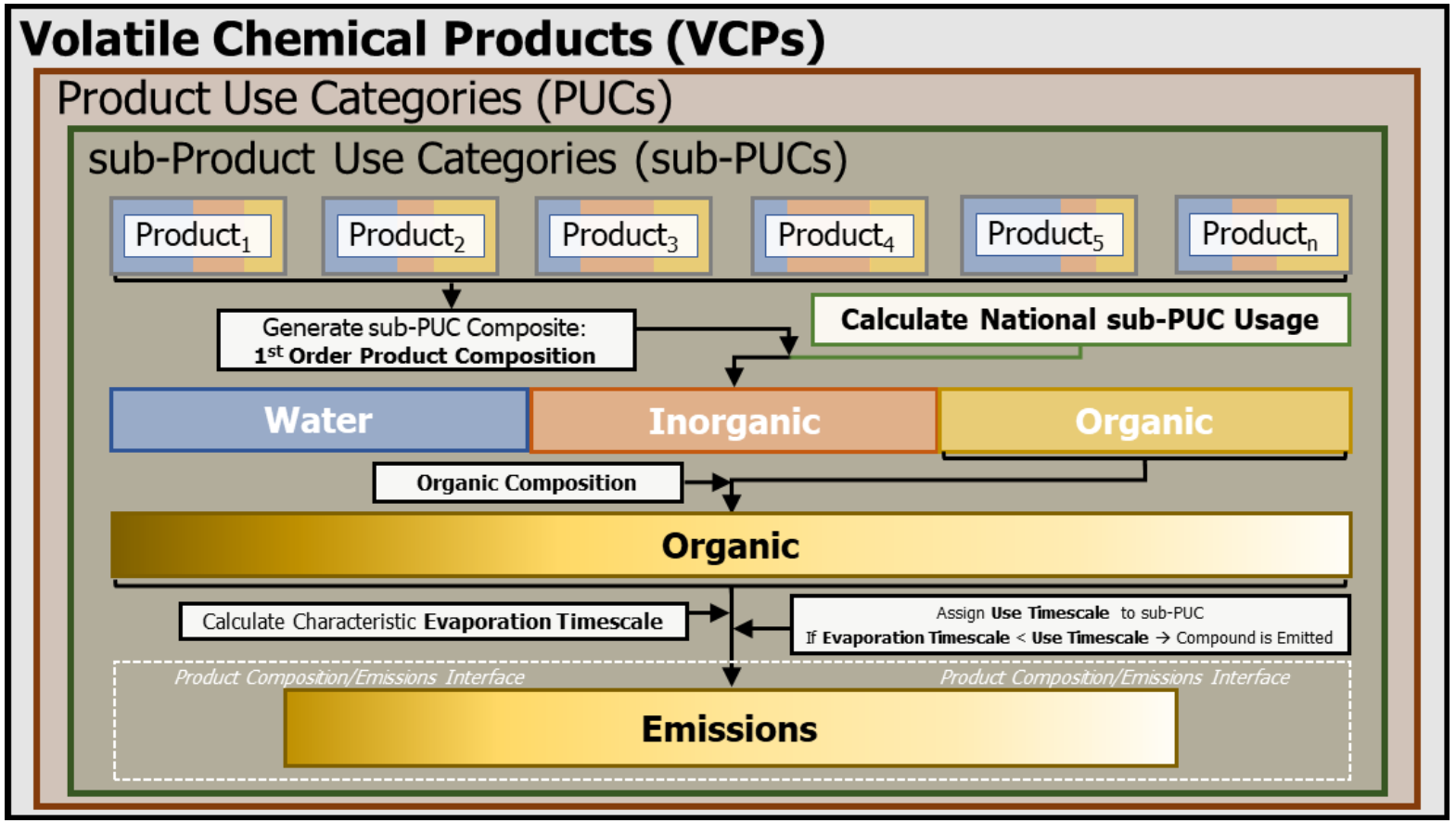
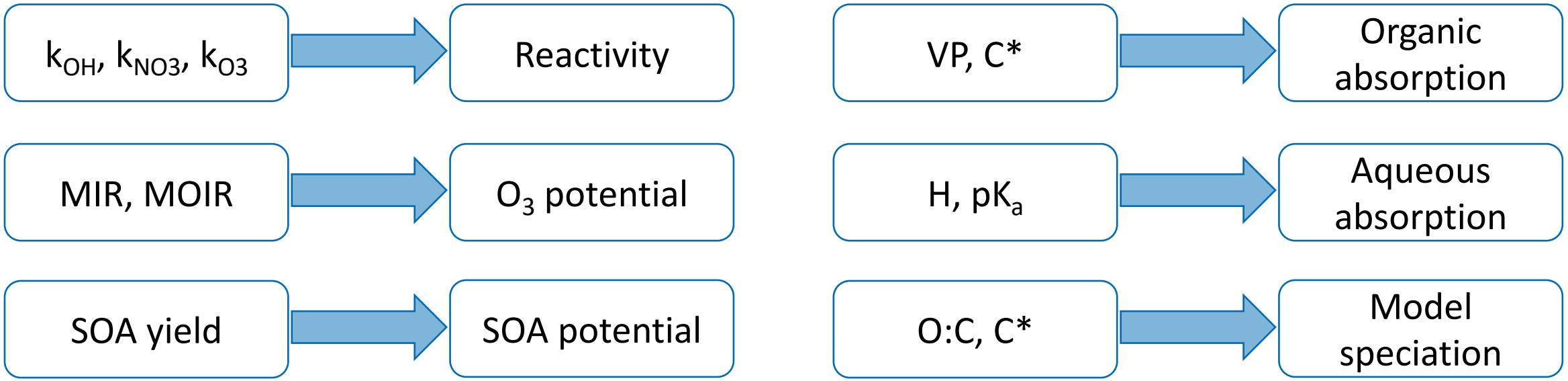
VCPy: a new emissions inventory



Seltzer et al., in prep

For more information, see Karl Seltzer's presentation: *Reactive Organic Carbon Emissions from Volatile Chemical Products*

VCPy species classified in terms of SOA



Data sources/QSAR models:

OPERA (Mansouri et al., 2018)
CompTox Chemicals Dashboard (Williams et al., 2017)
Chemical Transformation Simulator (Wolfe et al., 2016)

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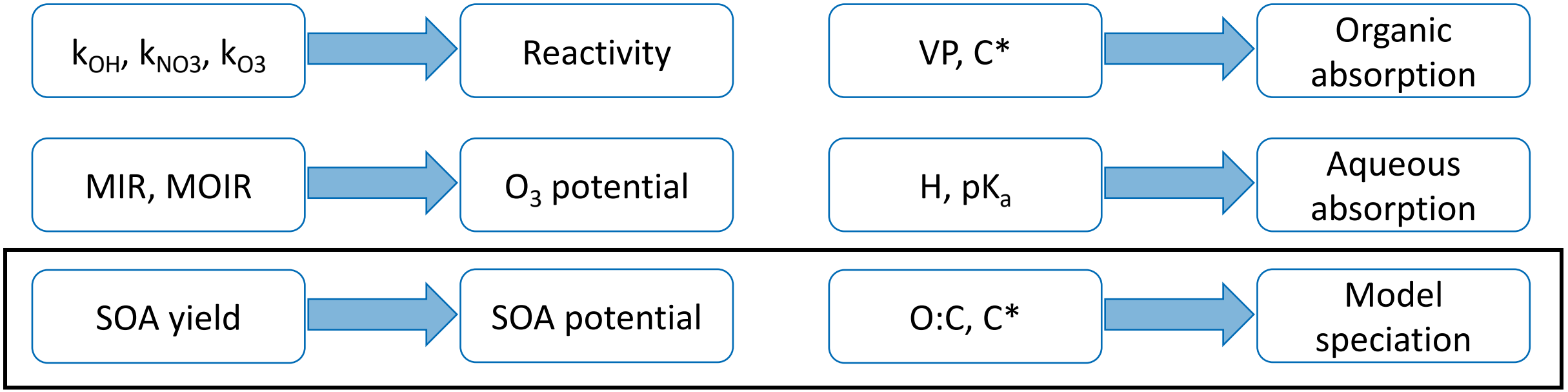

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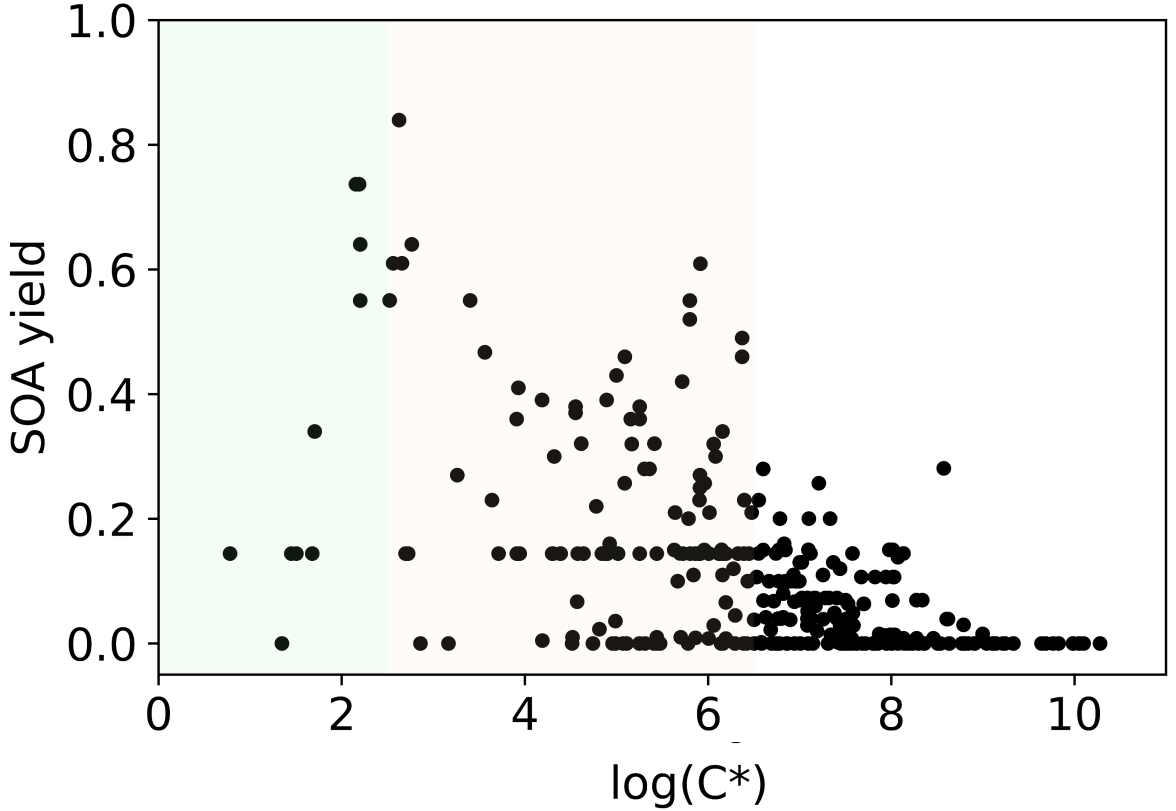
SOA yields

SOA yield 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)

Net SOA yield (weighted by location-specific emission rates):
LA County: 5.6%, CONUS: 5.3%



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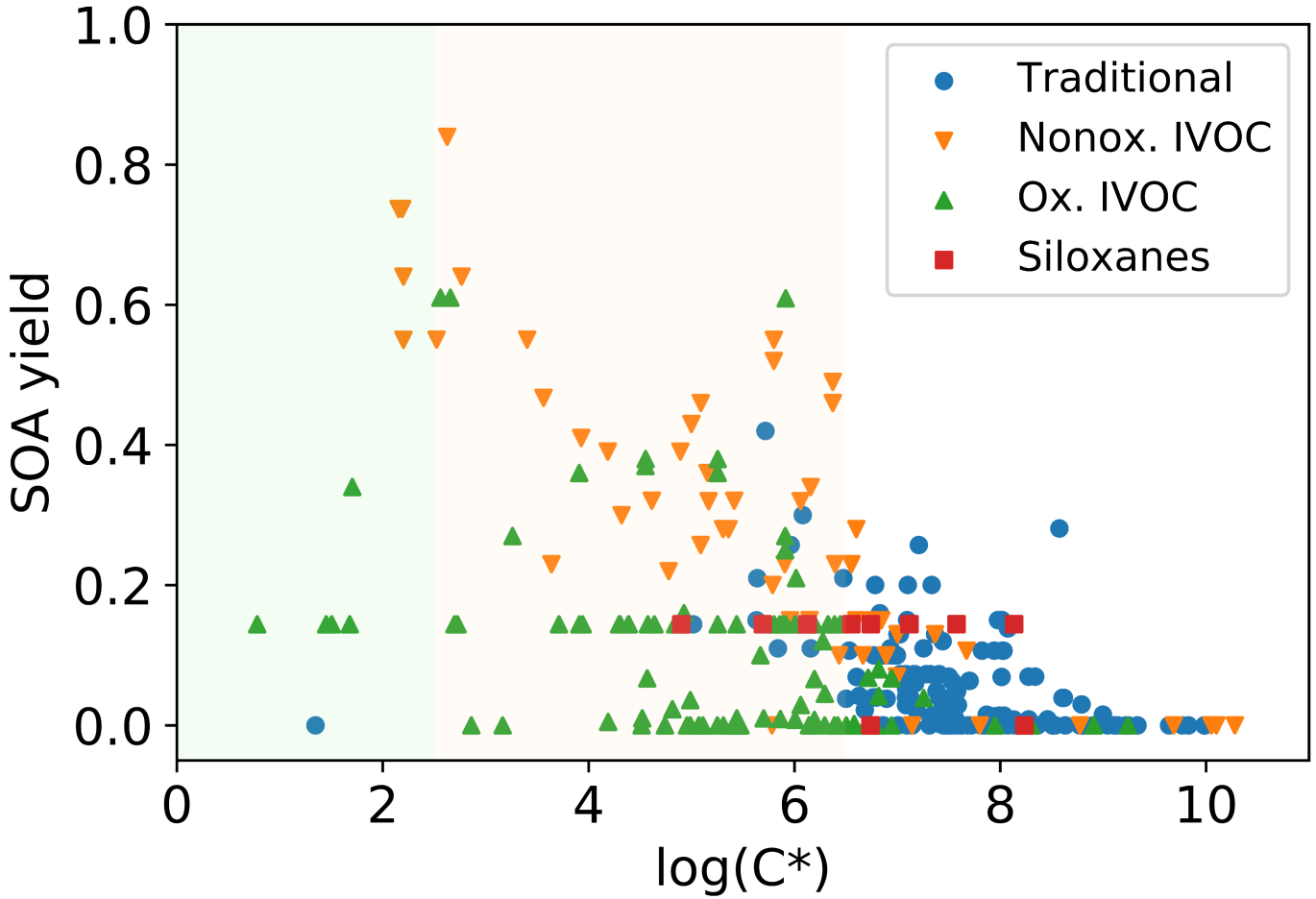
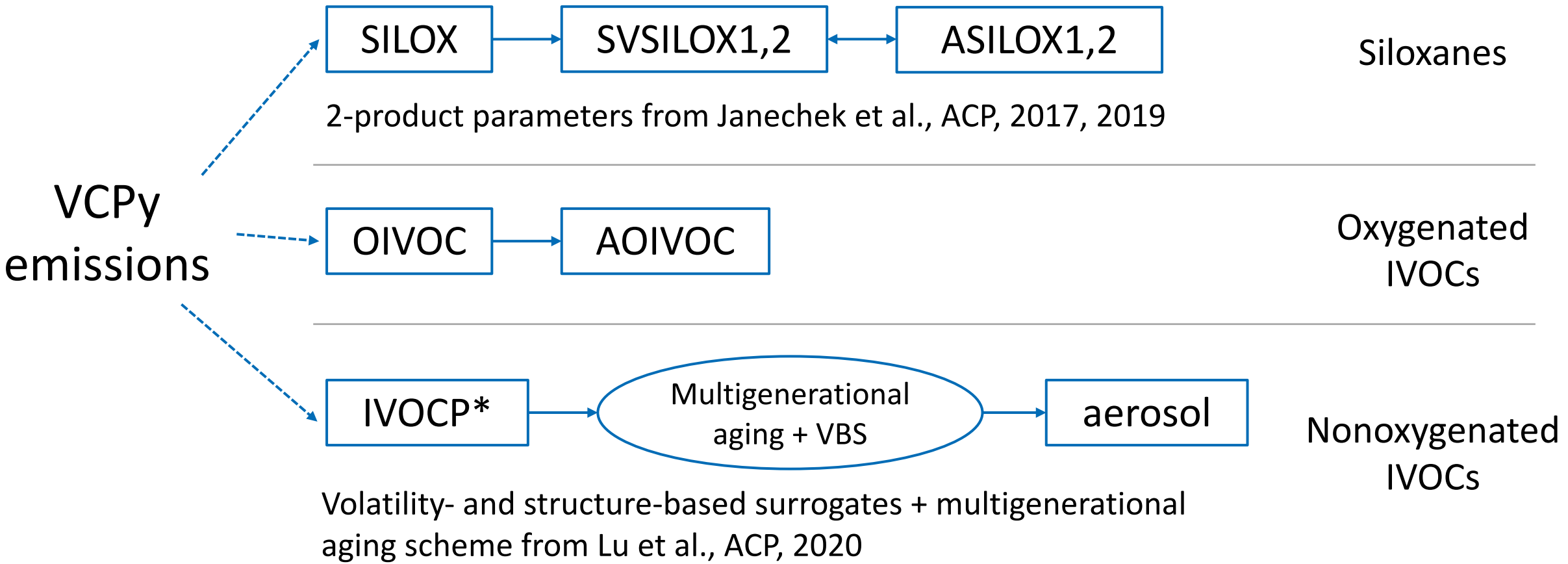
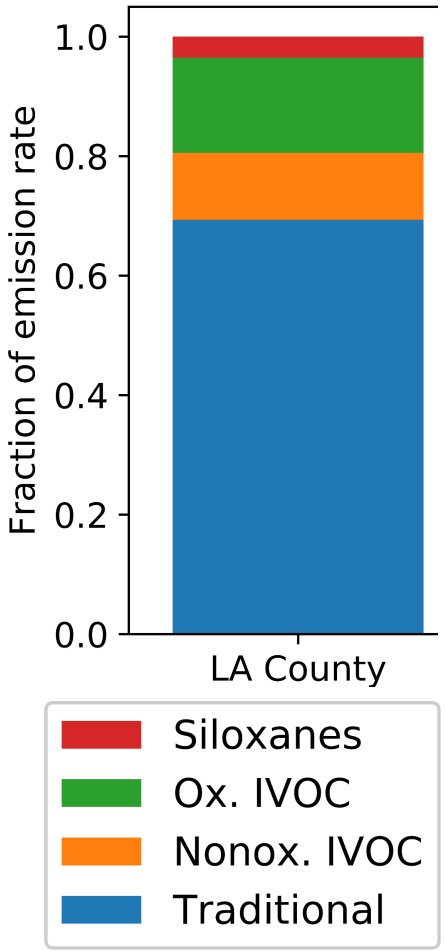
IVOC SOA yields fall in three classes



VCP chemical mechanism



VCP chemical mechanism



SILOX → SVSILOX1,2 ↔ ASILOX1,2

Siloxanes

2-product parameters from Janechek et al., ACP, 2017, 2019

OIVOC → AOIVOC

Oxygenated IVOCs

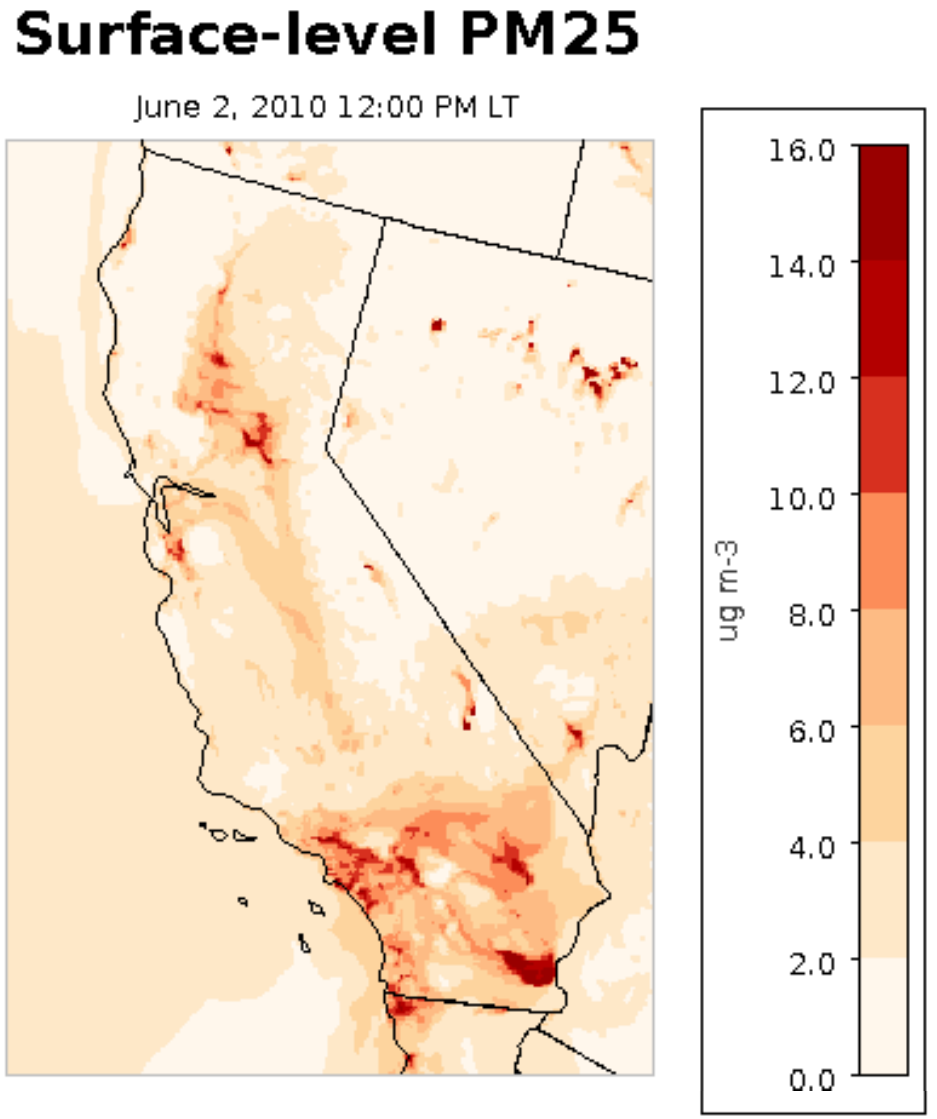
IVOCP* → Multigenerational aging + VBS → aerosol

Nonoxygenated IVOCs

Volatility- and structure-based surrogates + multigenerational aging scheme from Lu et al., ACP, 2020

Community Multiscale Air Quality (CMAQ) Model

- 3-D chemical transport model
- CMAQ version 5.3.2beta
- 4 km grid, 325 x 225 grid cells
- May 15 – June 15, 2010
- NEI 2011 emissions inventory
- WRF version 3.8.1 meteorology
- SAPRC07TC + aero7i



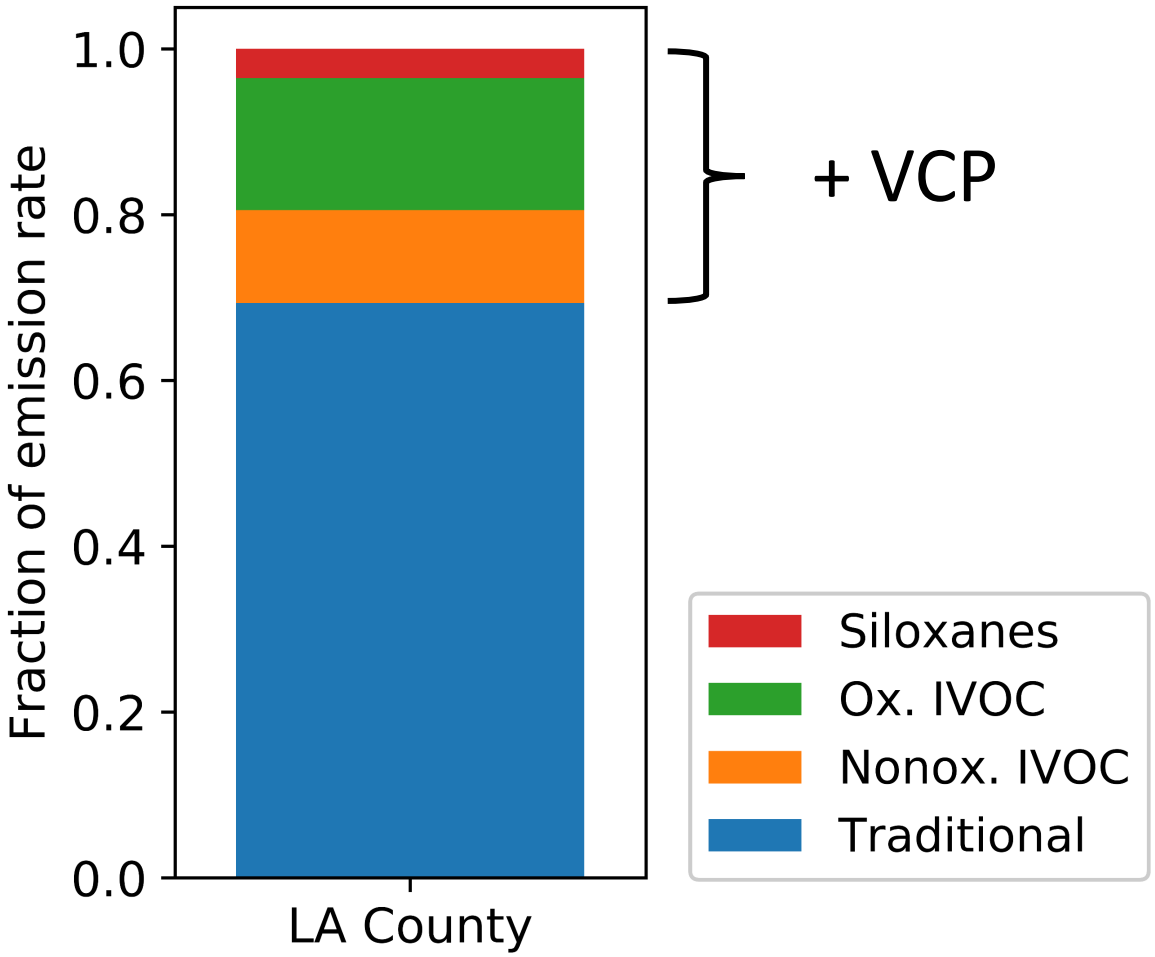
CMAQ simulations

Base

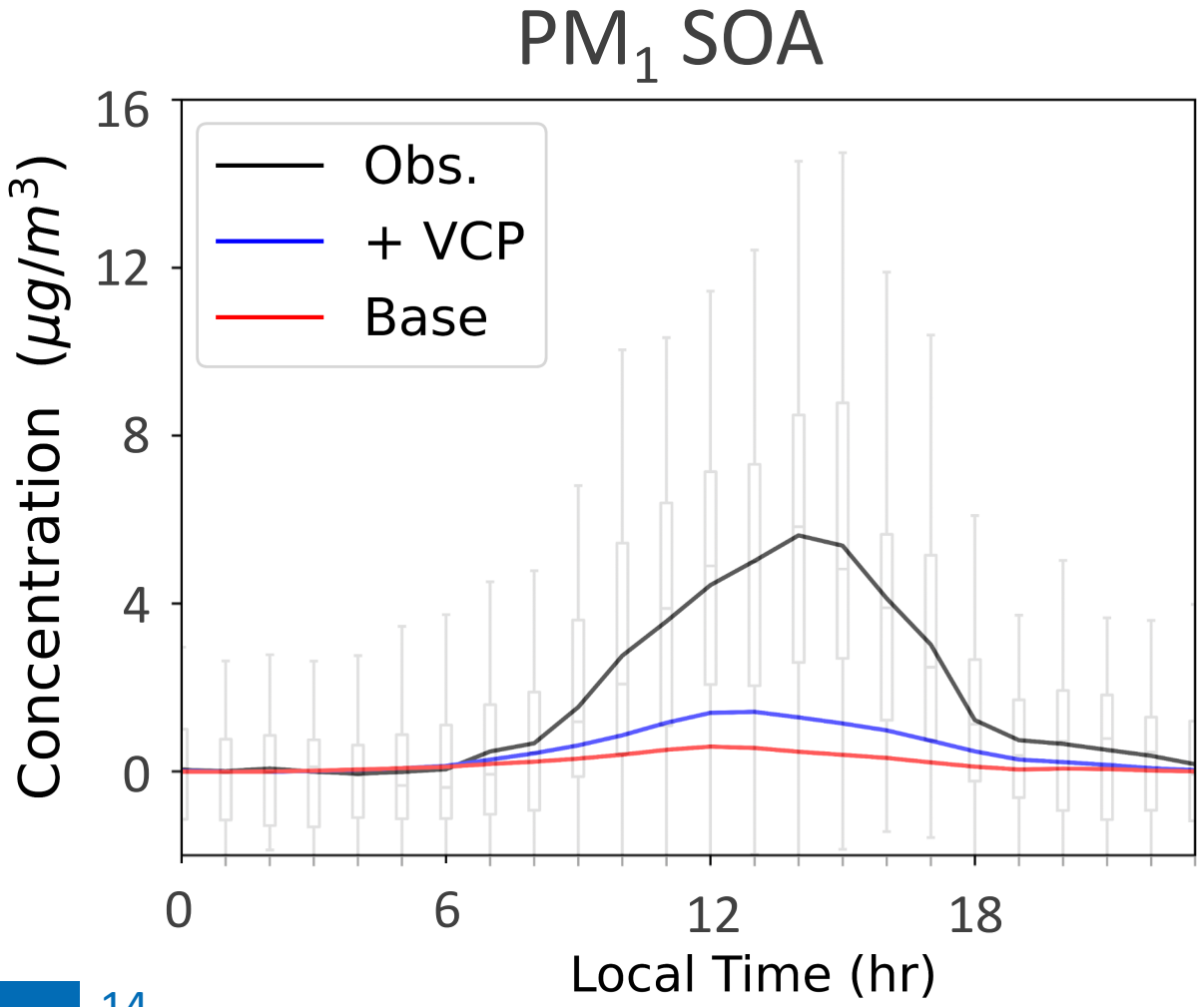
- EPA Calnex configuration
- pcSOA removed

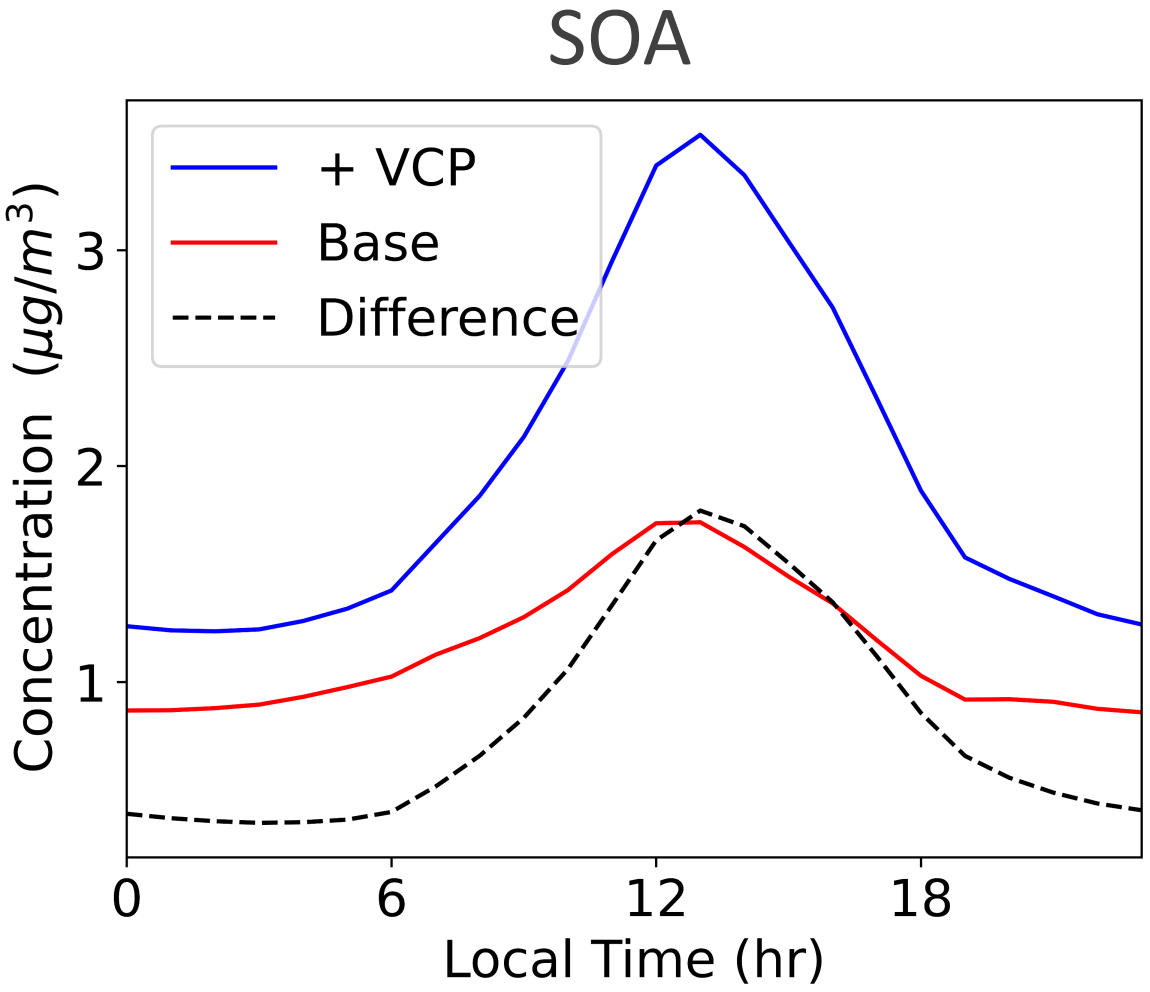
+ VCP

- Base + 3 new VCP IVOC pathways
- VCP IVOC emissions scaled to CO



IVOCs from VCPs add up to 2 µg/m^3





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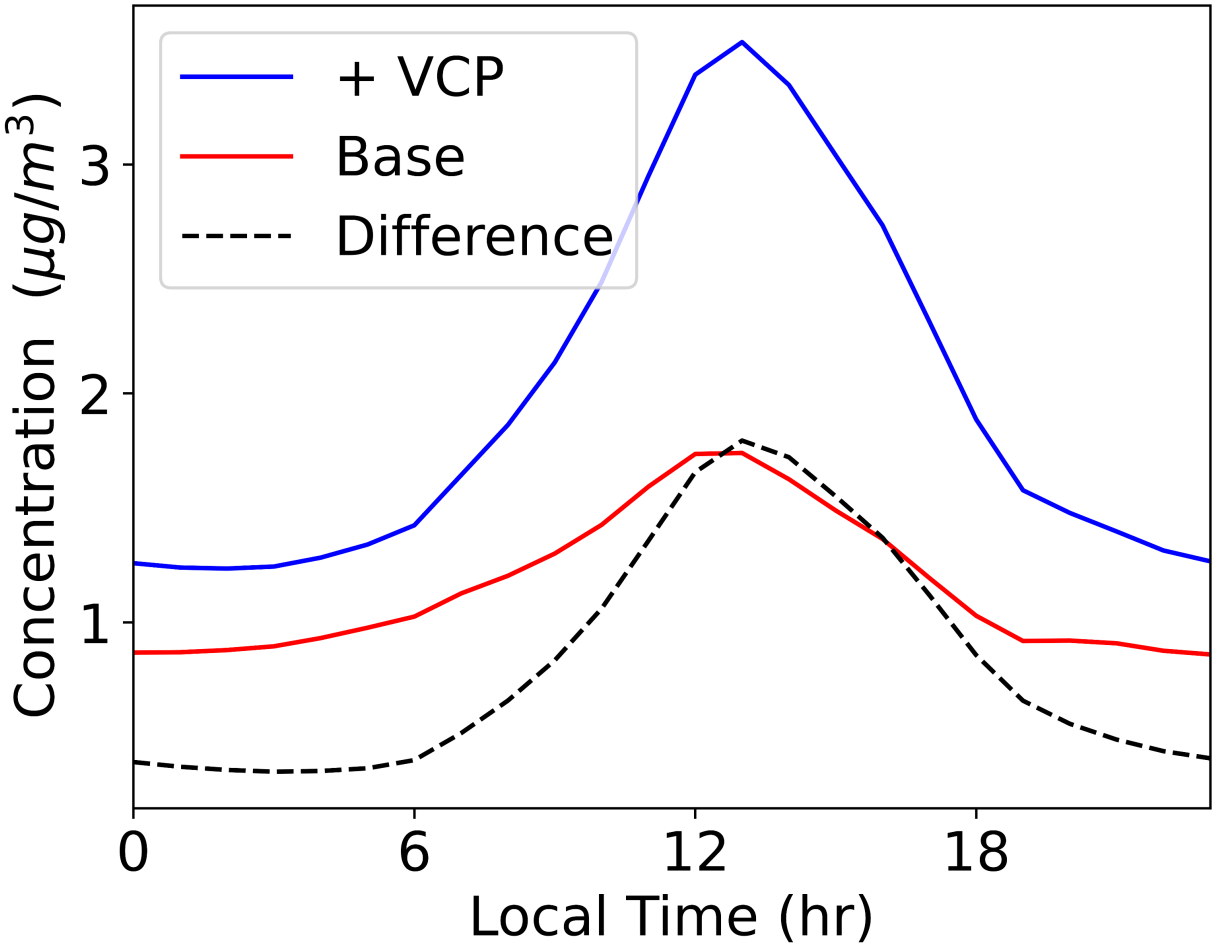

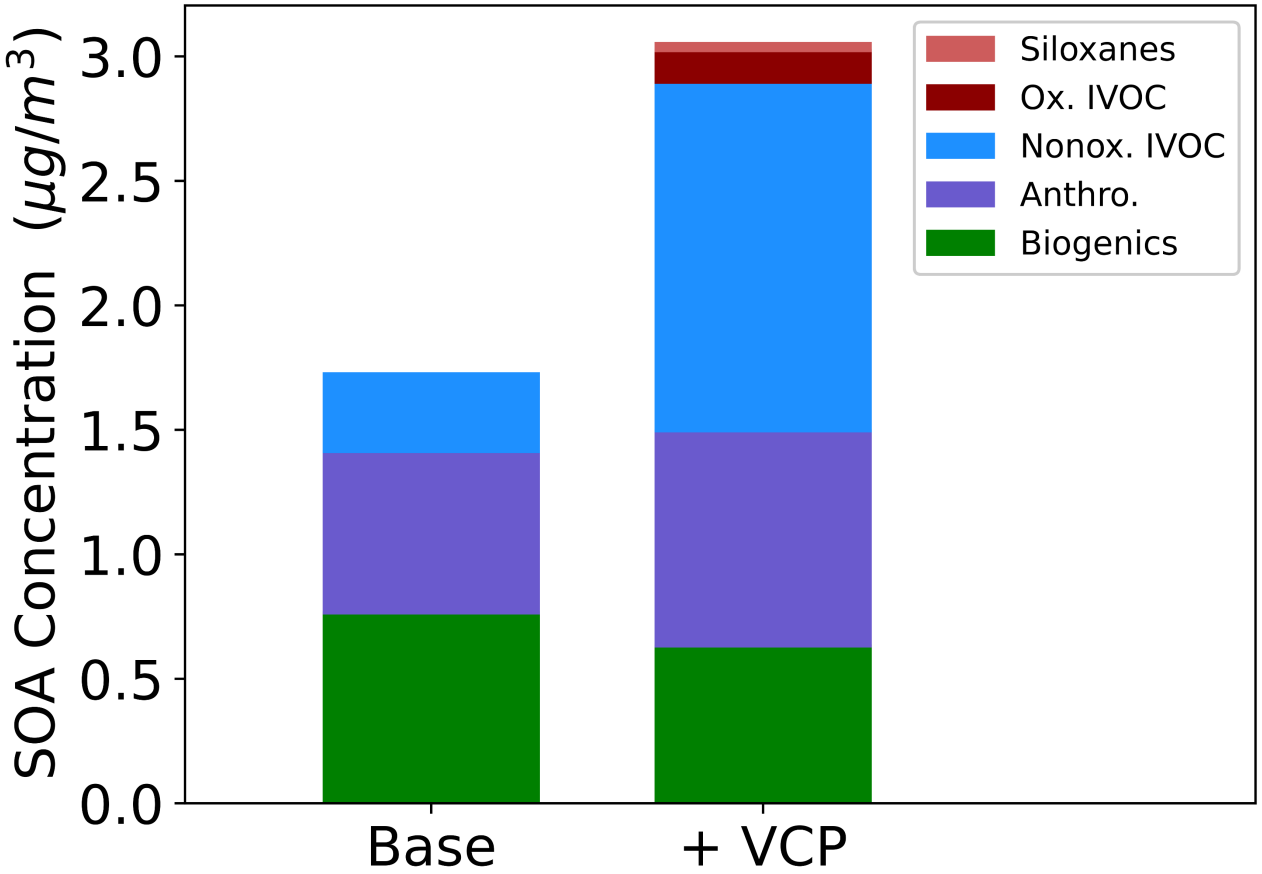

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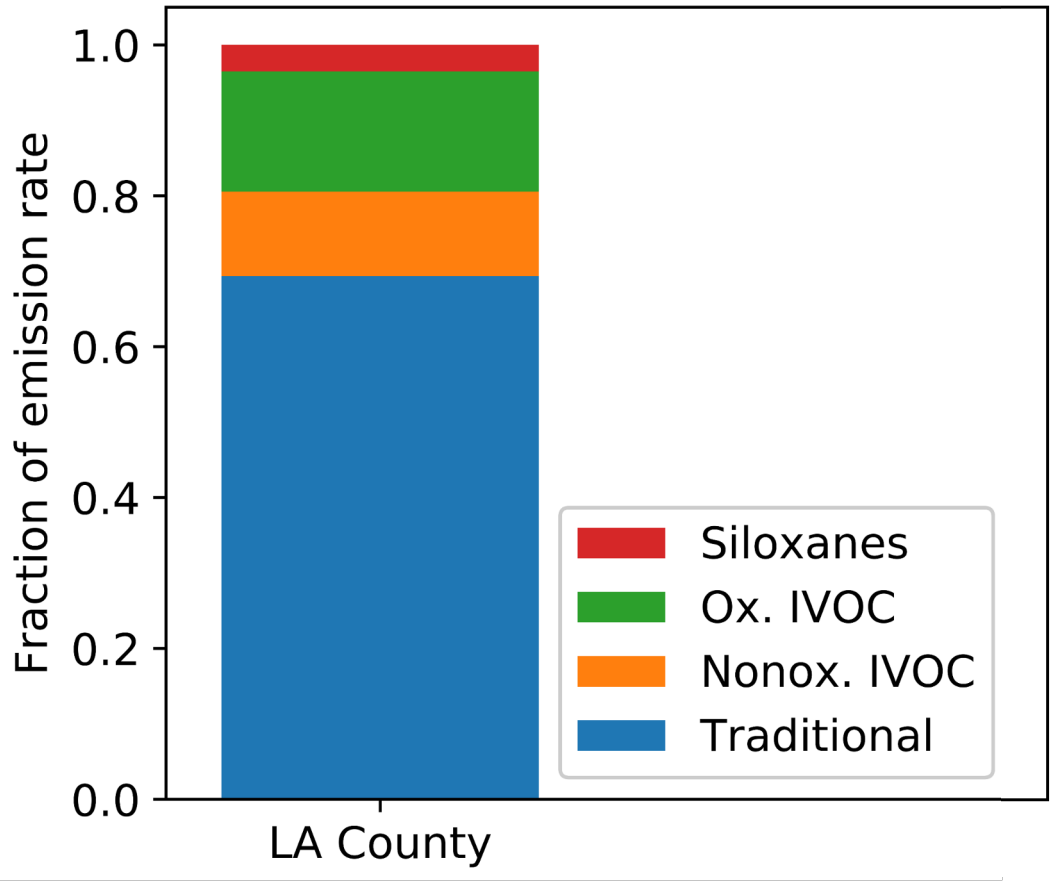

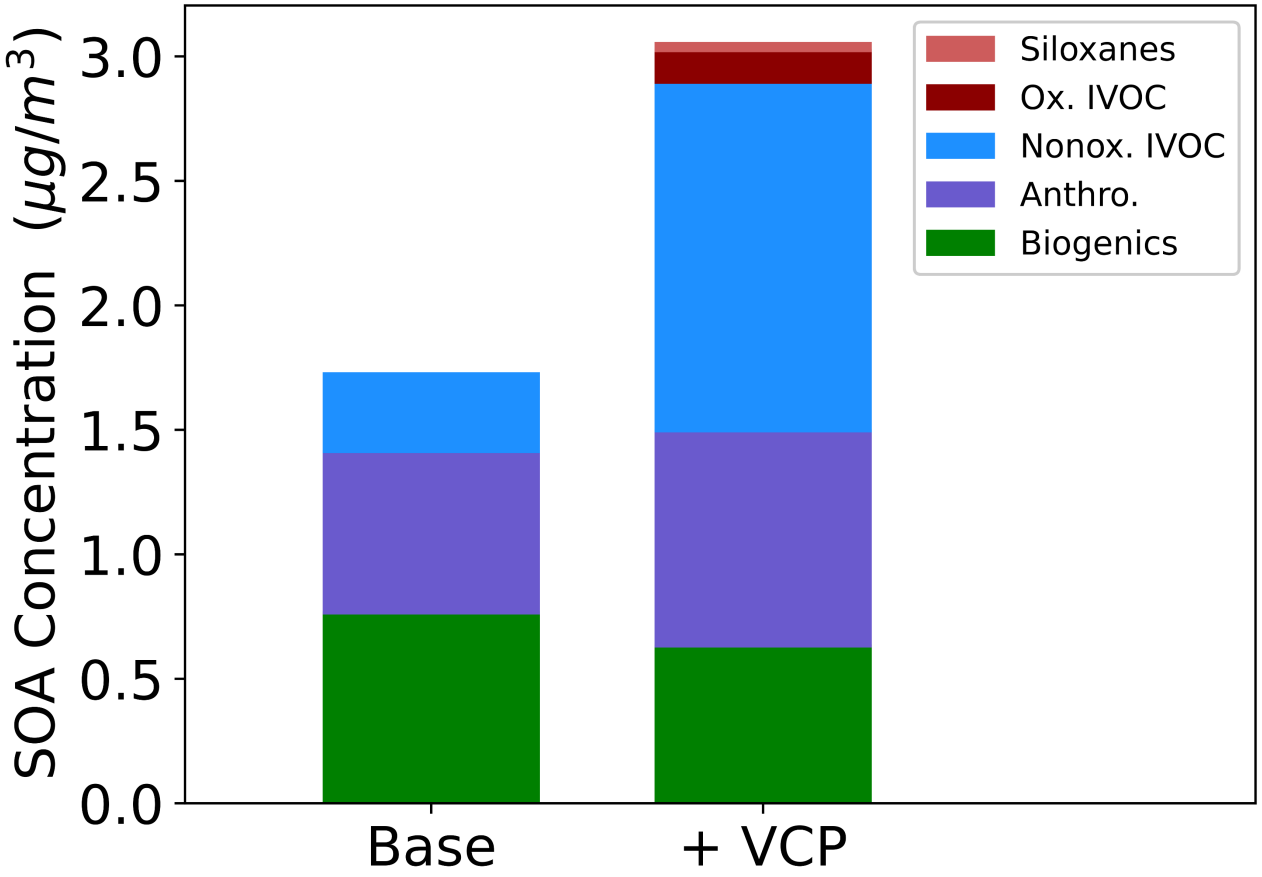

Conclusions

- Noontime SOA mass in CMAQ increased by up to 2 µg/m^3 as a result of improved representation of VCP IVOCs
- Siloxanes, oxygenated IVOCs, and nonoxygenated IVOCs have unique SOA yields and emission distributions and should be treated separately in CTMs
- Improved speciation profiles are necessary to better understand SOA formation from VCP VOCs

Future work

- Spatially and temporally allocated emissions inputs will be generated to provide more realistic diurnal profiles
- SOA yields for VCPs will be updated as more data become available through chamber and modeling studies

Acknowledgements

- The authors would like to thank Chris Cappa, Melissa Venechek, and Wyat Appel for their discussions on data development and analysis.
- Funding: EPA, ORISE, Samsung Global Research Outreach Award, JPL Visiting Student Researcher Program

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