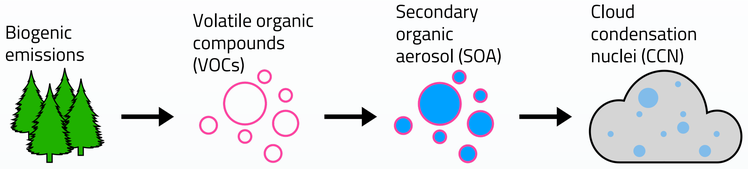
# Using laboratory data to inform superdroplet representations of surface-active organics

Clare E. Singer[1,2], Sylwester Arabas[3], Ryan X. Ward[1,4]

[1]California Institute of Technology, [2]now: NOAA GFDL, [3]AGH University of Krakow, [4]now: Columbia University

## Surface-active organics




When organic components preferentially partition to the surface of the aerosol, they alter both hygroscopicity (κ) and surface tension (σ).

$$S_{eq} = \left(\frac{r^3 - r_d^3}{r^3 - (1-\kappa)r_d^3}\right) \exp\left(\frac{2\,\sigma\,M_w}{RT\rho_w r}\right)$$

## Models of surface-partitioning

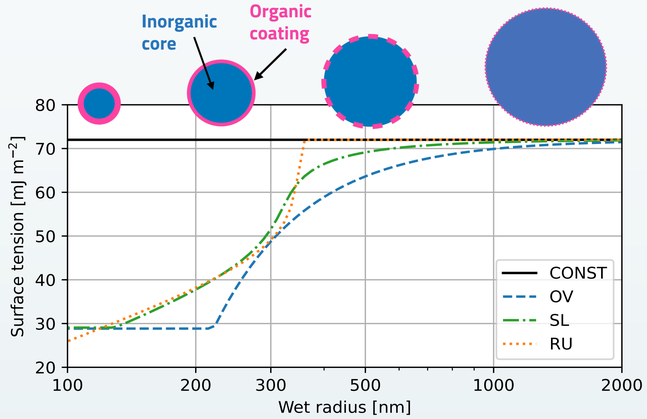
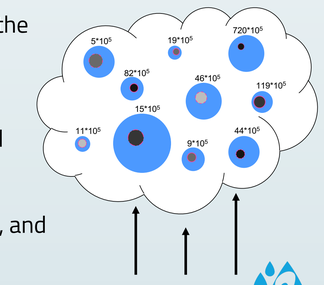



**Fig 1.** 3 models of surface-partitioning vary in complexity (from OV with 2 parameters to RU with 4). For SL and RU, organics can form a film on the surface which alters surface tension and dissolve into the bulk phase which alters hygroscopicity.

## PySDM

- Open-source, Pythonic implementation of the superdroplet method.
- Represents cloud particles (aerosols → precipitation) with few computational "superdroplets." Each has a multiplicity and physical attributes (dry radius, wet radius, hygroscopicity, organic fraction).
- Available in 0D (box or adiabatic parcel), 1D, and 2D kinematic configurations.



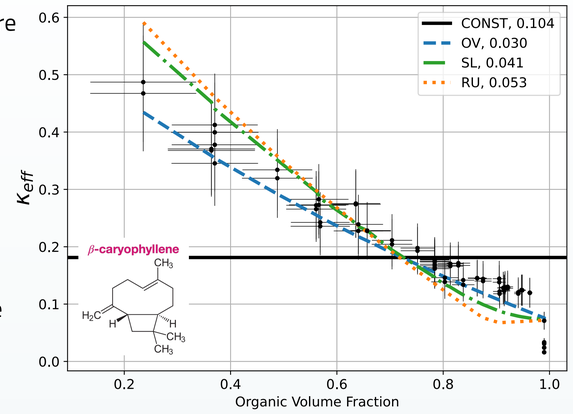
https://github.com/open-atmos/PySDM

- v1: Bartman, et al. *JOSS*, (2022), doi: 10.21105/joss.03219
- v2: de Jong, Singer, et al. *JOSS*, (2023, doi: 10.21105/joss.04968

PySDM

## Parameter calibration

Model parameters are fit using MCMC to minimize error with measured effective hygroscopicity, as shown in **Fig 2.** Results are for β-caryophyllene oxidized in dark conditions by ozone. Measurements were made in the Caltech flow tube reactor by Ryan Ward.




## Parcel model

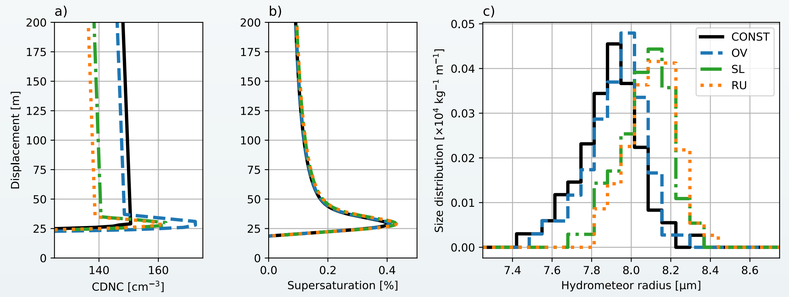



**Fig 3.** PySDM parcel model run with w=0.5 ms$^{-1}$, $N_a$=200 cm$^{-3}$, $r_a$=50nm, $F_{org}$=0.5. With best-fit parameters, the three models for surface-partitioning of organics give similar results. All models predict that including surface-partitioning yields fewer, larger cloud droplets (RU, SL, then OV in order from largest to smallest deviations from CONST).

## Parametric vs. Structural Uncertainty

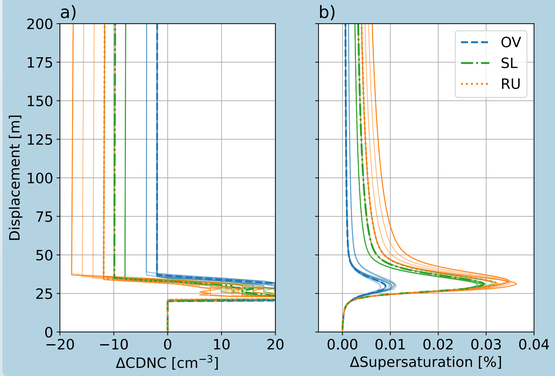
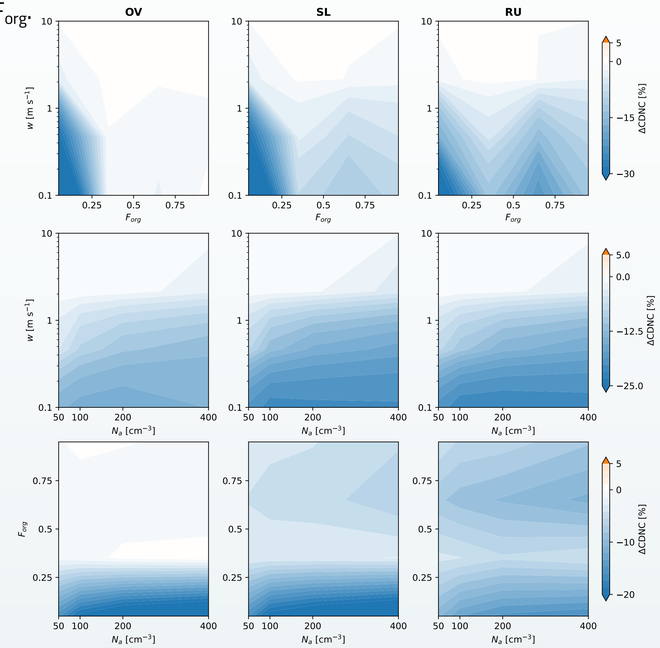



**Fig 4.** Varying the parameters for each surface tension model results in an ensemble of predictions, but structural differences are just as large as this spread.

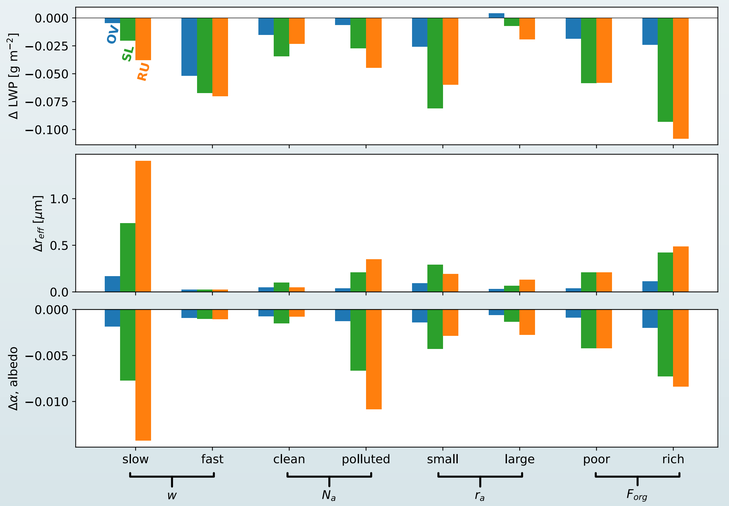
## Sensitivity to background conditions

**Fig 5.** ΔCDNC (compared to CONST) sensitivity to environmental and aerosol conditions (w, $F_{org}$, $N_a$). OV shows nearly no difference except at very small $F_{org}$. RU and SL both show a secondary peak of enhanced ΔCDNC for moderate $F_{org}$.




***What are the implications for cloud radiative effect?***

**Fig 6.** Difference in liquid water path (LWP), droplet effective radius ($r_e$), and cloud albedo (α) as compared to CONST surface tension. Surface-partitioning is most influential in *slow* updraft conditions, with *polluted* background aerosol concentration, and for *small* aerosols that are *rich* in organics.




Contact me: clare.singer@noaa.gov, claresinger.github.io