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Supplement of

Design and characterization of a new oxidation flow reactor for laboratory and long-term ambient studies

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S1. CFD simulations and RTD measurements

We coupled the Laminar Flow and the Transport of Diluted Species built-in modules and used a finite element method to simulate specific experimental conditions. The simulation geometry includes a diffuser inlet, reaction section, and cone outlet, all with exact dimensions. A finer mesh comprised of approximately 3.59×10^6 tetrahedral elements was applied to the entire three-dimensional model to capture flow dynamics near the entrance to the exit cone. An impermeable and no-slip boundary condition was applied to all surfaces. The inlet flow to the reactor was prescribed to be 3.5 L min^{-1} and the outlet pressure was assumed to be atmospheric. The simulations were run until a steady state was achieved and the errors converged to $< 10^{-5}$.

S2. LVOCs fate correction

Here, the method developed by Palm et al. (2016) was used to correct for losses due to: (1) condensation on the reactor wall, (2) exiting the reactor, and (3) reacting with OH.

The equations are shown below:

$$\tau_{aerosol} = \frac{1}{4\pi \times CS \times D} \tag{1}$$

$$CS = \sum_i r_i \beta_i N_i \tag{2}$$

$$\beta = \frac{K_n + 1}{0.377K_n + 2 + \frac{4}{3}\alpha^{-1}K_n^2 + \frac{4}{3}\alpha^{-1}\frac{4}{3}\alpha^{-1}K_n} \tag{3}$$

$$K_n = 3\sqrt{\frac{\pi M}{8RT}}\frac{D}{r} \tag{4}$$

$$\tau_{wall} = \frac{\pi}{2\frac{A}{V}\sqrt{k_e D}} \tag{5}$$

$$k_e = 0.004 + 0.0056 \cdot V^{0.74} \tag{6}$$

$$\tau_{OH} = \frac{5}{k_{OH} \cdot [OH]} \tag{7}$$

$$\frac{1}{\tau_{total}} = \frac{1}{\tau_{wall}} + \frac{1}{\tau_{OH}} + \frac{1}{\tau_{aerosol}} \tag{8}$$

$$F_{exit} = e^{-\frac{\tau_{OFR}}{\tau_{total}}} \tag{9}$$

$$F_{aerosol} = (1 - F_{exit}) \cdot \frac{\tau_{total}}{\tau_{aerosol}} \tag{10}$$

$$F_{wall} = (1 - F_{exit}) \cdot \frac{\tau_{total}}{\tau_{wall}} \tag{11}$$

$$F_{OH} = (1 - F_{exit}) \cdot \frac{\tau_{total}}{\tau_{OH}} \tag{12}$$

Where:

D —the diffusion coefficient, which is estimated to be 7×10^{-6} m^2 s^{-1} for oxidized organic vapor with a molecular weight of 200 g mol^{-1} (Tang et al., 2015)

CS —the condensation sink calculated from the particle size distribution

r_i and N_i — the particle radius and number concentration of each size bin of the SMPS

β —the correction factor for gaseous diffusion to the particle surface

α— the mass accommodation coefficient (also known as the sticking coefficient) of condensing vapor, which is assumed to be 1

Kn —the Knudsen number

M — the molecular weight of the condensing vapor, which is assumed to be 200 g mol^{-1}

A/V —the surface-area-to-volume ratio, which is 0.53 cm^{-1} for the PFA OFR

k_e — the eddy diffusion coefficient

k_{OH} — rate constant for reaction with OH, which is assumed to be 1×10^{11} cm^3 $molec^{-1}$ s^{-1}

Figures and Tables

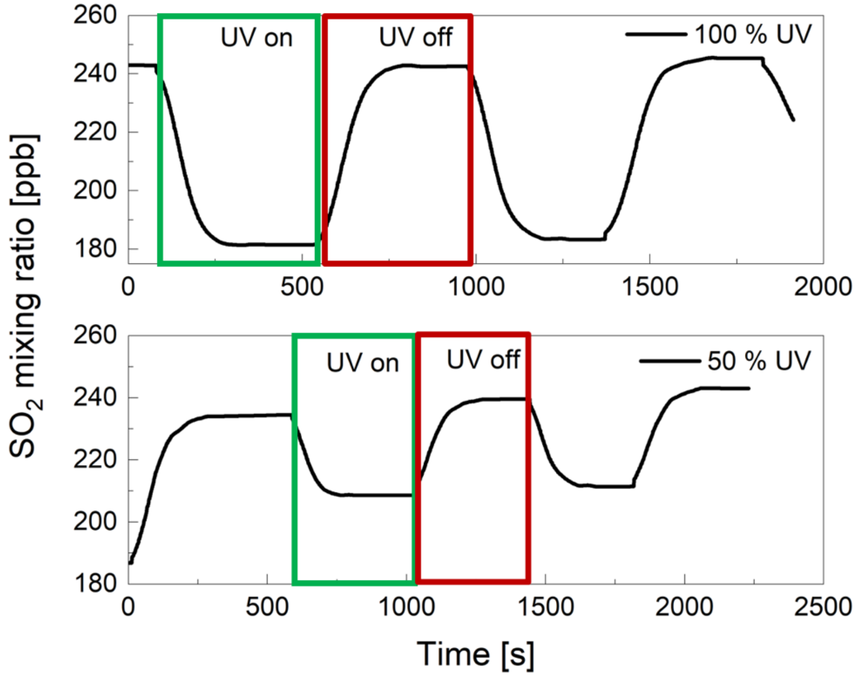

Figure S1: Example results from experiments to characterize OH exposure using injected SO_2.

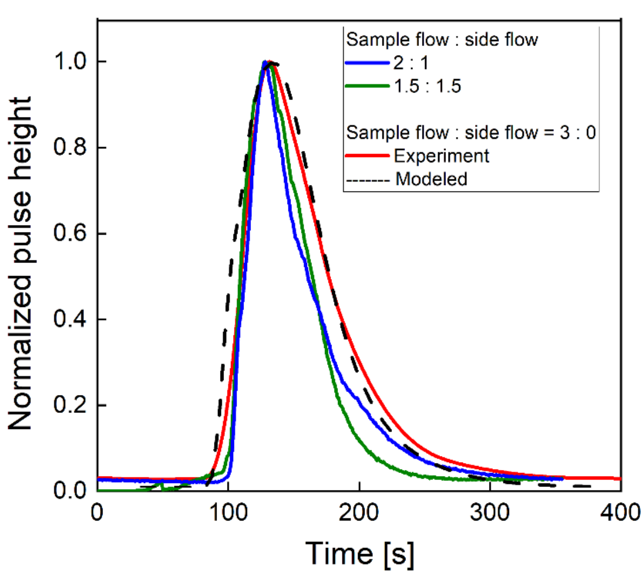

Figure S2: Measured response of pulse injection of AS particles with the side purge flow on (blue and green solid line) and off (red solid line), and the COMSOL simulation of the configuration with it turned off (black dashed line).

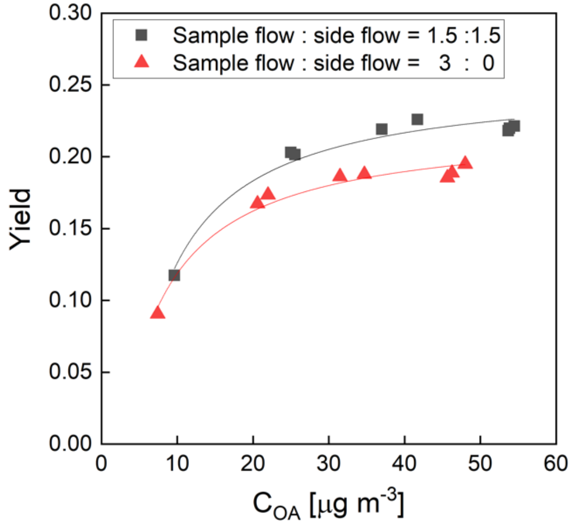

Figure S3: α-pinene SOA yield as a function of organic aerosol concentration (C_{OA}) generated in the PFA OFR at a estimated OH exposure of 3 × 10^{11} molec. cm^{-3} s. Measured SOA yield with the side purge flow on (black squares) and off (red triangles).

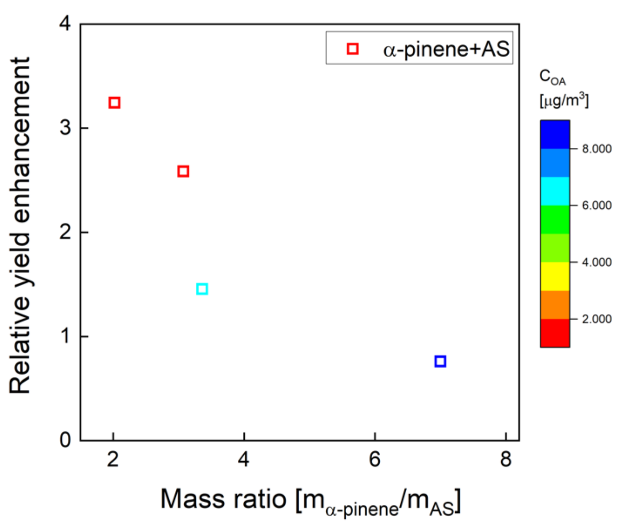

Figure S4: Relative α-pinene SOA yield enhancement as a function of the mass ratio of α-pinene and AS seed particles. Marker color reflects aerosol mass concentration.