Supporting Information for Simulation of organic aerosol formation during the CalNex study: updated emissions and simplified secondary organic aerosol parameterization for intermediate volatility organic compounds

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1 Parameter fitting for SOA formation from lumped IVOC species

The loss term is defined as squared error between two surfaces: $m_{SOA,simp}(OA,t)$ and $m_{SOA,79}(OA,t)$:

$$Loss = \Sigma_{OA=1}^{10}\Sigma_{t=1}^{48}(m_{SOA,simp}(OA,t) - m_{SOA,79}(OA,t))^2 \quad (1)$$

which minimizes the squared distances between two surfaces in (OA concentration, time) space. Due to very high non-linearity in Eq. (1), the optimization is decoupled into step 1: 'kOH fitting' and step 2: 'SOA yield fitting'.

Step 1: Relax the constrain on SOA yield to fit kOH, Eq. (2) can be rewritten as,

$$m_{SOA,simp}(t) = \sum_j m_j\, \gamma_j f\left(k_{OH,j},t\right) = \sum_j m_j\, \gamma_j (1 - \mathrm{e}^{-k_{OH,j}[OH]\Delta t}) \quad (2)$$

where γ_j is the free variable representing SOA yield of surrogate j at given OA concentration, [OH] is assuming to be 3×10^6 cm^{-3}. Solving Eq. (2) with 2 unknowns: $k_{OH,j}$ and γ_j, $k_{OH,j}$ is the fitted OH reaction rate for the new lumped IVOC group.

Step 2: After solving for $k_{OH,j}$, we now eliminate the non-linearity in the time term of Eq. (2) by replacing unknown $f\left(k_{OH,j},t\right)$ with calculated reacted fraction $r_{j,t} = 1 - \mathrm{e}^{-k_{OH,j}[OH]\Delta t}$ from fitted $k_{OH,j}$. Therefore, we can minimize the loss in Eq. (1) for each reduced IVOC groups,

$$Loss = \Sigma_{OA=1}^{10}\Sigma_{t=1}^{48}(\sum_{i\in j} m_{SOA,i}\,(OA,t) - \sum_{i\in j} m_{IVOC,i}\left[\alpha_{j,1}\xi_{OA,C^*=0.1} + \alpha_{j,2}\xi_{OA,C^*=1} + \alpha_{j,3}\xi_{OA,C^*=10} + \alpha_{j,4}\xi_{OA,C^*=100}\right] r_{j,t})^2 \quad (3)$$

where $\alpha_{j,1}$ to $\alpha_{j,4}$ are the fitted SOA parameterization for reduced IVOC group j. Minimization of the loss between $m_{SOA,simp,j}(OA,t)$ to $\sum_{i\in j} m_{SOA,i}\,(OA,t)$ is performed with the surface fitting toolbox in MATLAB.

2 Figs. S1 to S4

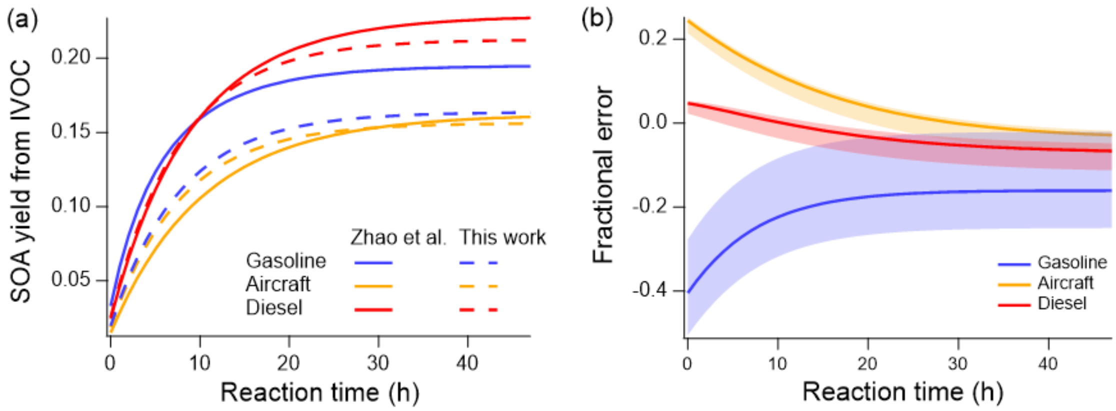

Figure S1: (a) Comparison of predicted SOA formation per unit mass mobile IVOC emission using original and four-lumped-species parameterizations at OA = 5 μg m^{-3}, average [OH] = 3 × 10^6 cm^{-3} (b) Relative error in SOA formed between original and four-lumped-species parameterizations (Solid line is the relative error at OA = 5 μg m^{-3}, shaded area corresponds to OA = 1 to 50 μg m^{-3})

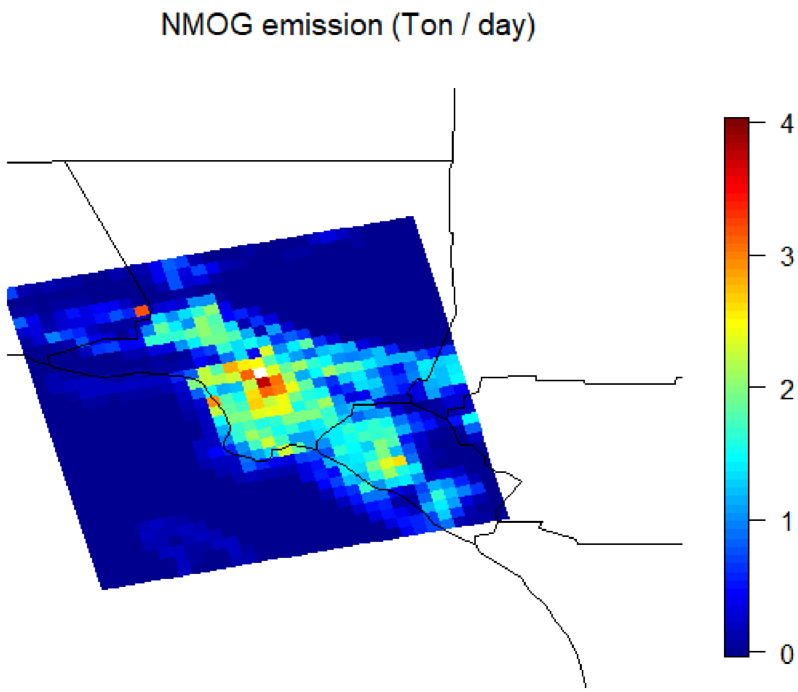

Figure S2: (a) Los Angeles region in this study as defined by simulation grid cells (30 × 30 grid cell with 4 km resolution, equivalent to 120 km × 120 km)

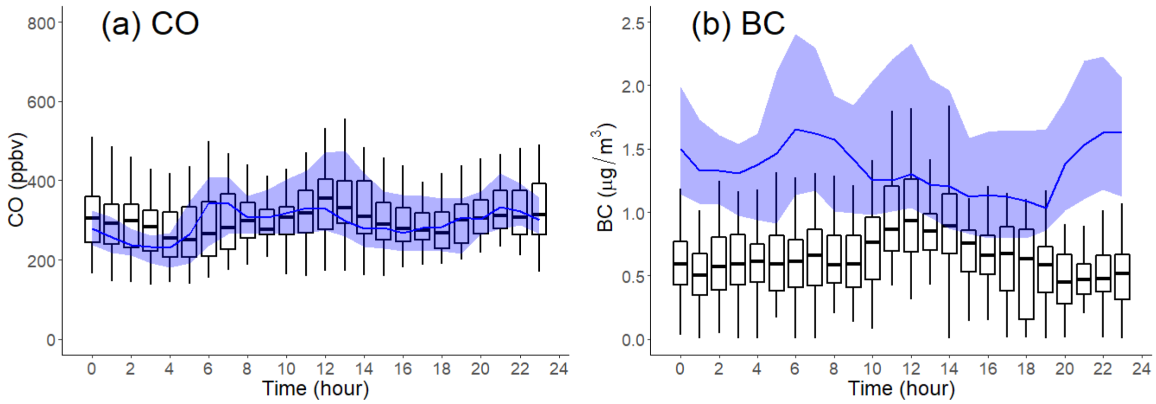

Figure S3: Comparison of measured (boxplot, solid box denotes 25th to 75th percentiles and whiskers denote 10th to 90th percentiles) and modelled (line, shaded area denotes 25th to 75th percentiles) diurnal patterns in Pasadena, CA during CalNex for species: (a) CO (b) BC

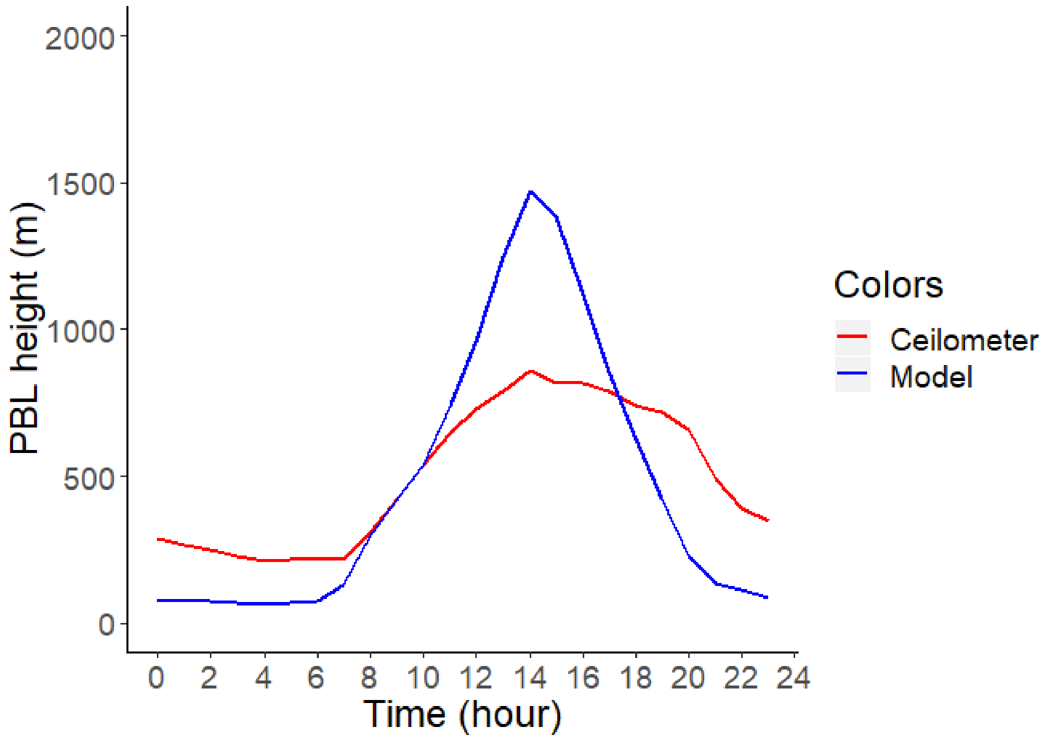

Figure S4: Comparison of ceilometer measured (h1) and modelled PBL height diurnal patterns at Pasadena during CalNex (line denotes median value)