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Supplement of

GECKO-A v1.0: exploring VOC oxidation trajectories through comparison with the master chemical mechanism

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S1 Priority scheme for surrogate (isomer) selection

When the "isomerfg" option is enabled, a newly generated species can be replaced by a positional isomer already present in the mechanism. The two species must share the same molecular formula and the same set of functional groups. Substitution is restricted to non-radical species with more than four carbon atoms, beyond the second generation only. The newly generated species must also have a formation yield below 3%. If several matching isomers exist, the following structural criteria are applied in order. At each step, only isomers meeting the criterion are retained. If no isomer meets it, the current list remains unchanged and the next criterion is applied.

1. Carbon skeleton branching pattern (relative numbers of primary, secondary, tertiary, and quaternary carbon nodes)
2. Number of –CO–CO– conjugated pairs
3. Number of 1,2-interactions between functional groups
4. Number of terminal CH_3 groups
5. Presence of long terminal alkyl chains, checked from longest (four-carbon) to shortest (two-carbon)
6. Number of –CO–CO– pairs located at a chain terminus
7. Number of 1,4-interactions, followed by 1,3-interactions between functional groups
8. Number of specific –CO–CHO, –CO–C(O)OONO$_2$, –CO–C(O)OH, and –CO–C(O)OOH conjugated pairs
9. Number of CH_2, CH, and C carbon types, in that order

If, after all criteria have been applied, more than one isomer still matches, the isomer already present in the mechanism with the highest Ymax is selected.

S2 Thermodynamic phase partitioning – boundary lines in the phase partitioning space

Let C_g, C_w, and C_o denote the molar concentrations of a species X in the gas phase, aqueous phase, and organic particulate phase, respectively, per liter of air. In what follows, absorption into condensed phases is modeled using a simplified framework: absorption into the organic condensed phase is described by Raoult's law, while absorption into the aqueous phase follows Henry's law. Under these laws, the behavior of species is assumed to be ideal, and the organic and aqueous phases are treated as immiscible.

■ Gas/Aqueous Phase Partitioning

The equilibrium between the gas and aqueous phases for species X is governed by Henry's Law:

$$H = \frac{[X]}{p_X}$$

where H (M.atm^{-1}) is the Henry's law coefficient, $[X]$ is the aqueous-phase concentration of X (in M), p_X is its partial pressure (in atm). Introducing ω_L, the liquid water mixing ratio (volume of liquid water per volume of air), and expressing p_X using the ideal gas law, the phase partitioning ratio is given by:

$$\frac{C_w}{C_g} = HRT\omega_L$$

where R is the ideal gas constant ($R = 0.082$ L atm K^{-1} mol^{-1}).

The Henry's law constant at equipartition ($C_w/C_g = 1$) is:

$$H^{(g:w)} = \frac{1}{RT\omega_L}$$

■ Gas/Organic Particulate Phase Partitioning

The equilibrium between the gas and organic particulate phases follows Raoult's Law:

$$p_X = x_X^o \cdot p_{sat}$$

where x_X^o is the mole fraction of X in the organic phase, and p_{sat} is its saturation vapor pressure. Given C_{OA} as the mass concentration of organic particulate matter (µg/m³) and M_{OA} as the average molar mass (g/mol) of its constituents, the mole fraction is: $x_X^o = 10^{-9}\, C_O(M_{OA}/C_{OA})$ where the factor 10^{-9} accounts for unit conversions. Expressing p_X using the ideal gas law, the phase partitioning ratio is:

$$\frac{C_o}{C_g} = \frac{10^{-9}C_{OA}}{M_{OA}} \cdot \frac{RT}{p_{sat}}$$

The saturation vapor pressure at equipartition ($C_o/C_g = 1$) is:

$$p_{sat}^{(g:o)} = \frac{10^{-9}RT \cdot C_{OA}}{M_{OA}}$$

■ Aqueous/Organic Particulate Phase Partitioning

The equilibrium between the aqueous and organic particulate phases results from the two preceding equilibria. The partitioning ratio is:

$$\frac{C_w}{C_o} = \frac{10^{-9}\omega_L M_{OA}}{C_{OA}} \cdot H \cdot p_{sat}$$

The Henry's law constant at equipartition ($C_w/C_o = 1$) is:

$$H^{(w:o)} = \frac{10^{-9}C_{OA}}{\omega_L M_{OA}} \cdot \frac{1}{p_{sat}}$$

or equivalently:

$$H^{(w:o)} = H^{(g:w)} \cdot p_{sat}^{(g:o)} \cdot \frac{1}{p_{sat}}$$

■ Fraction in the Organic Particulate Phase

Let f_o be the fraction of X in the organic particulate phase:

$$f_o = \frac{C_o}{C_g + C_w + C_o} \implies \frac{1}{f_o} = 1 + \frac{C_g}{C_o} + \frac{C_w}{C_o}$$

Substituting the partitioning ratios, we obtain:

$$\frac{1}{f_o} = 1 + \frac{M_{OA}RT}{10^{-9}C_{OA}} \cdot p_{sat} + \frac{\omega_L M_{OA}}{10^{-9}C_{OA}} \cdot H \cdot p_{sat}$$

$$\frac{1}{f_o} = 1 + \frac{p_{sat}}{p_{sat}^{(g:o)}} + \frac{H \cdot p_{sat}}{H^{(g:w)} \cdot p_{sat}^{(g:o)}}$$

The boundary line $H = f(p_{sat})$ for a fixed f_o in the phase partitioning space is:

$$H = H^{(g:w)} \cdot \frac{(1 - f_o)}{f_o} \cdot \frac{p_{sat}^{(g:o)}}{p_{sat}} - H^{(g:w)}$$

■ **Fraction in the Aqueous Phase**

Let f_w be the fraction of X in the aqueous phase:

$$f_w = \frac{C_w}{C_g + C_w + C_o} \Longrightarrow \frac{1}{f_w} = 1 + \frac{C_g}{C_w} + \frac{C_o}{C_w}$$

Substituting the partitioning ratios, we obtain:

$$\frac{1}{f_w} = 1 + \frac{1}{HRT\omega_L} + \frac{C_{OA}}{10^{-9}\omega_L M_{OA}} \cdot \frac{1}{H \cdot p_{sat}}$$

$$\frac{1}{f_w} = 1 + \frac{H^{(g:w)}}{H} + \frac{H^{(g:w)}}{H} \cdot \frac{p_{sat}^{(g:o)}}{p_{sat}}$$

The boundary line $H = f(p_{sat})$ for a fixed f_w is:

$$H = H^{(g:w)} \cdot \frac{f_w}{1 - f_w} \cdot \left(1 + \frac{p_{sat}^{(g:o)}}{p_{sat}}\right)$$

■ **Fraction in the Gas Phase**

Let f_g be the fraction of X in the gas phase:

$$f_g = \frac{C_g}{C_g + C_w + C_o} \Longrightarrow \frac{1}{f_g} = 1 + \frac{C_w}{C_g} + \frac{C_o}{C_g}$$

Substituting the partitioning ratios, we obtain:

$$\frac{1}{f_g} = 1 + \frac{H}{H^{(g:w)}} + \frac{p_{sat}^{(g:o)}}{p_{sat}}$$

The boundary line $H = f(p_{sat})$ for a fixed f_g is:

$$H = \frac{1 - f_g}{f_g} \cdot H^{(g:w)} - \frac{p_{sat}^{(g:o)}}{p_{sat}} \cdot H^{(g:w)}$$

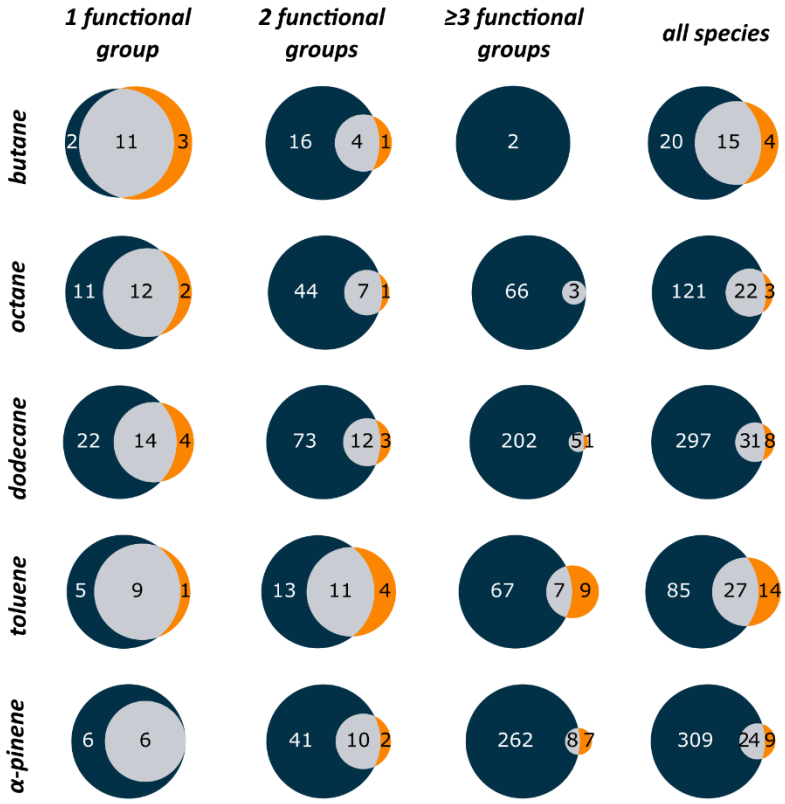


Figure S1: Number of non-radical isomer groups contributing to the carbon budget in the **urban** scenario, partitioned by presence in GECKO-A only, MCM only, or both mechanisms. Left to right panels: monofunctional isomers, bifunctional isomers, polyfunctional isomers (more than two functional groups) and all isomer groups. Top to bottom panels: butane, octane, dodecane, toluene, and α-pinene as parent compounds. Blue: isomer groups present only in GECKO-A; orange: isomer groups present only in MCM; gray: isomer groups common to both mechanisms.

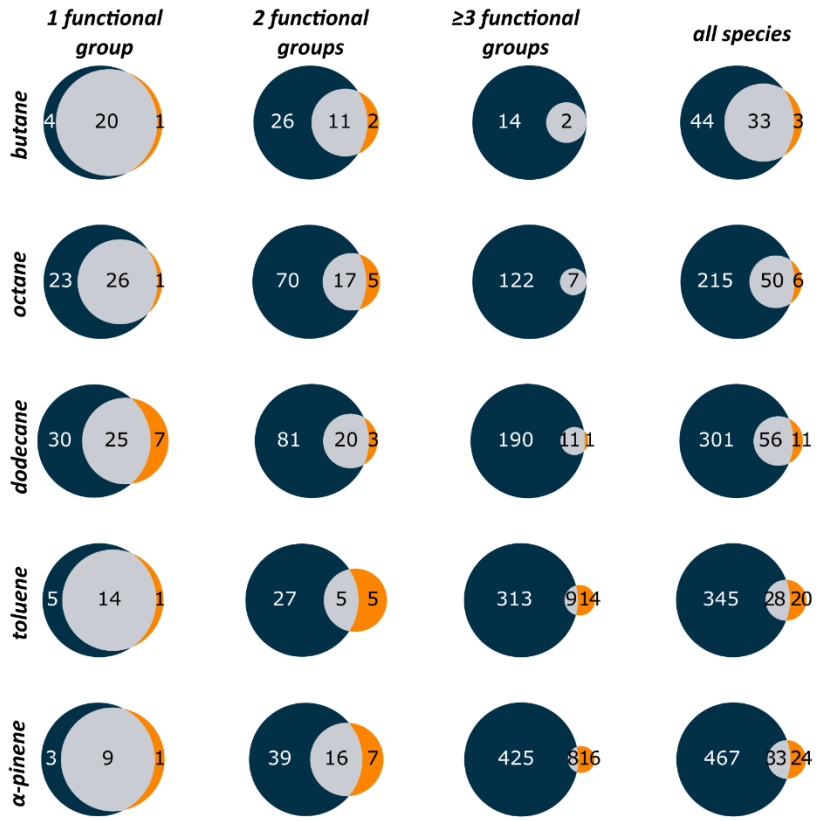


Figure S2: Number of non-radical isomer groups contributing to the carbon budget in the **remote** scenario, partitioned by presence in GECKO-A only, MCM only, or both mechanisms. Left to right panels: monofunctional isomers, bifunctional isomers, polyfunctional isomers (more than two functional groups) and all isomer groups. Top to bottom panels: butane, octane, dodecane, toluene, and α-pinene as parent compounds. Blue: isomer groups present only in GECKO-A; orange: isomer groups present only in MCM; gray: isomer groups common to both mechanisms.

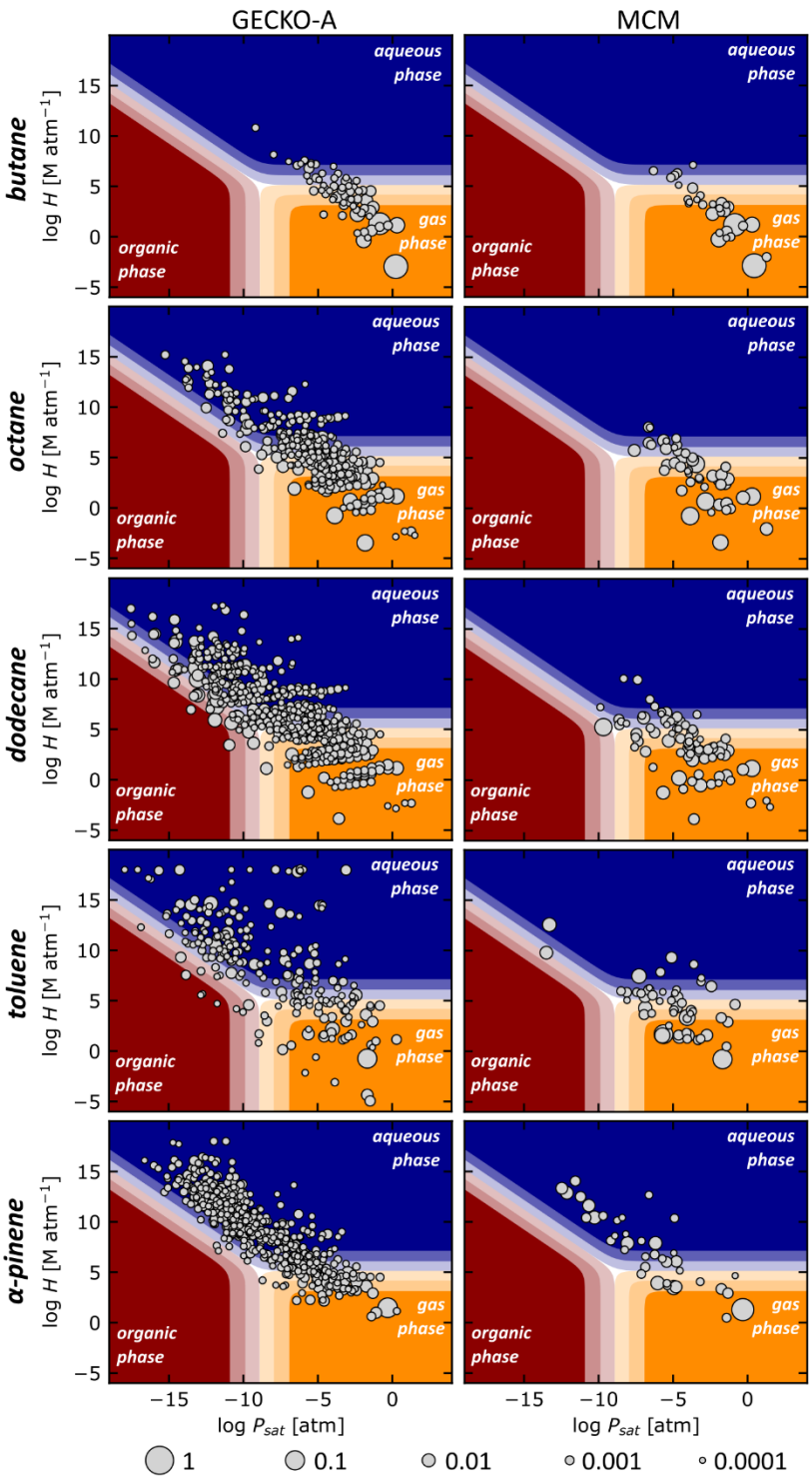


Figure S3: As Figure 15 in the main text, but for a cloud liquid water environment. Distribution of species from GECKO-A (left column) and MCM (right column) as a function of their saturation vapor pressure and effective Henry's law constant, for the continental scenario after 72 hours of simulation. From top to bottom: butane, octane, dodecane, toluene, and α-pinene as parent compounds. Colored domains indicate the dominant phase of each species at thermodynamic equilibrium: dark, intermediate, and light shades representing partitioning greater than 99%, 90%, and 50% in the respective phase. Domain boundaries are calculated for a mass concentration of 10 µg/m³ in the organic particulate phase and a liquid water mixing ratio $\omega_L = 3 \times 10^{-7}$. Bubble size represents the relative carbon abundance of each species normalized to the initial parent compound.

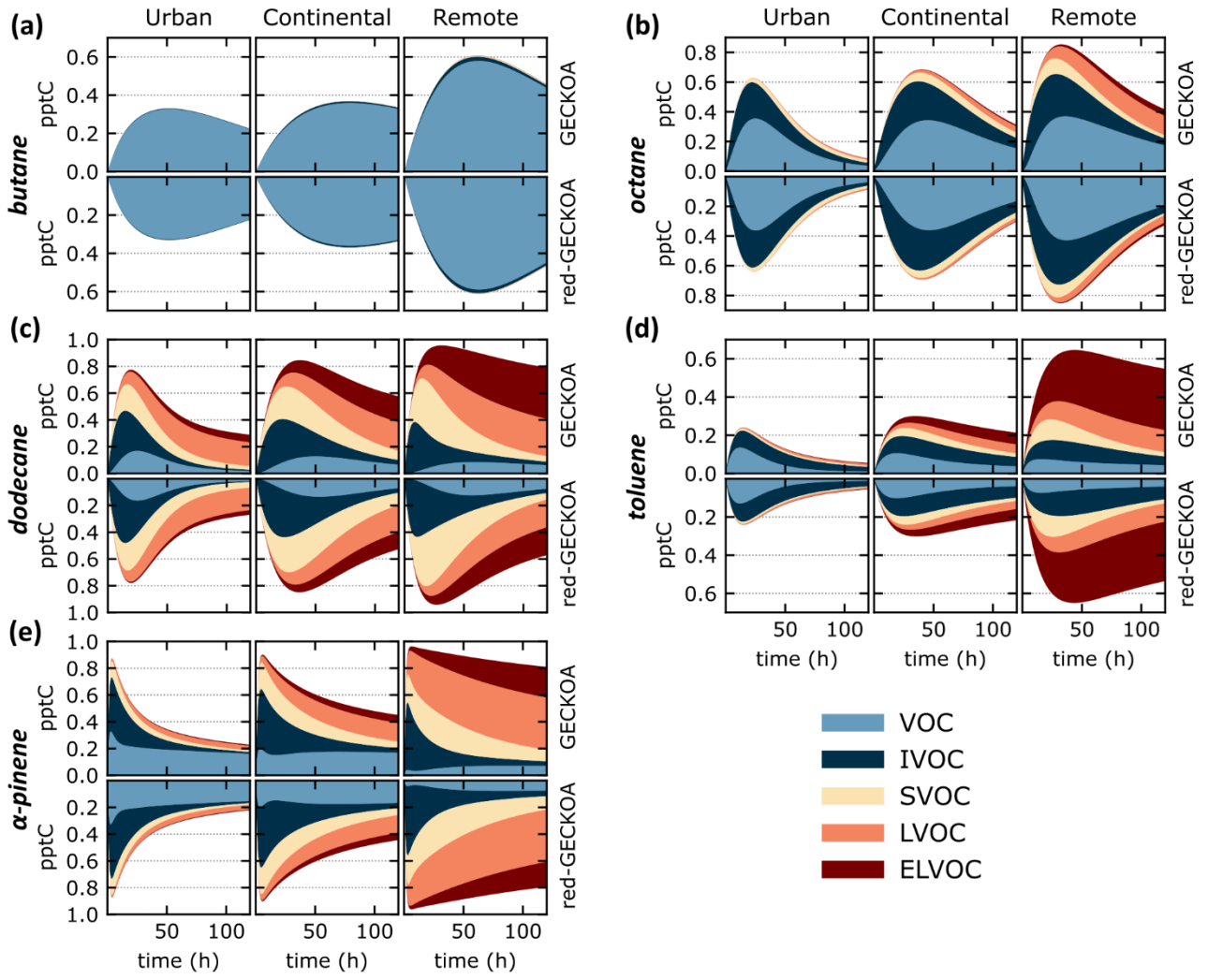


Figure S4: Temporal evolution of secondary organic carbon (SOC) by volatility group for various parent hydrocarbons under different environmental scenarios. Panels (a–e): butane, octane, dodecane, toluene, and α-pinene as parent hydrocarbons, respectively. From left to right in each panel: urban, continental, and remote scenarios. Top and bottom lines in each panel: GECKO-A and red-GECKO-A simulation results, respectively. Color code: light blue (VOC), dark blue (IVOC), yellow (SVOC), orange (LVOC), red (ELVOC).

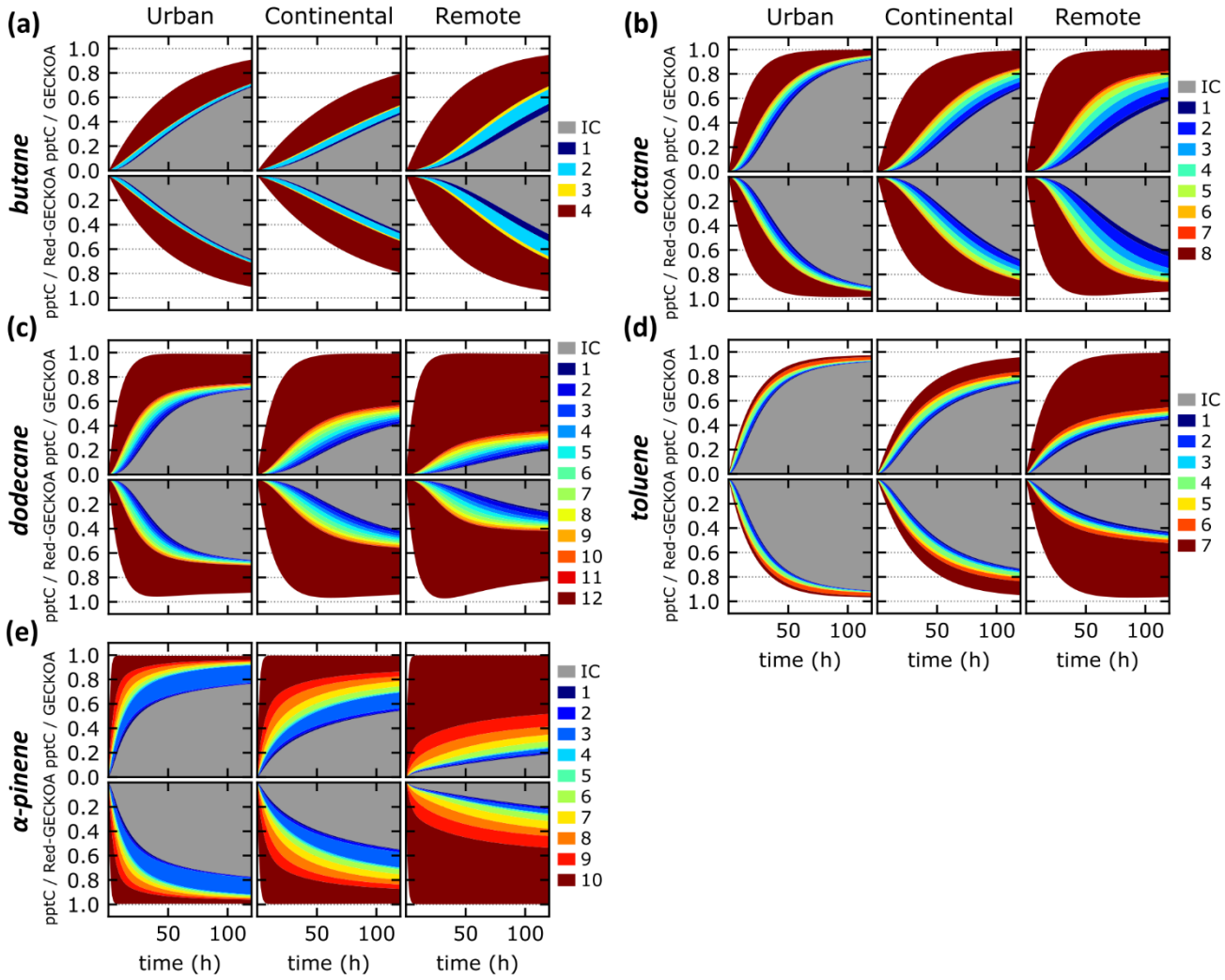


Figure S5: Temporal evolution of secondary carbon summed across gas and particle phases and grouped by carbon chain length for various parent hydrocarbons under different environmental scenarios. Panels (a–e): butane, octane, dodecane, toluene, and α-pinene as parent hydrocarbons, respectively. From left to right in each panel: urban, continental, and remote scenarios. Top and bottom rows in each panel: GECKO-A and red-GECKO-A simulation results, respectively. The color gradient indicates the number of carbon atoms in the species, with dark red representing organic species with carbon chain lengths equal to the parent hydrocarbon, dark blue representing organic C_1 species, and intermediate colors for chain lengths in between. The gray color is for secondary inorganic carbon (IC = CO + CO_2).

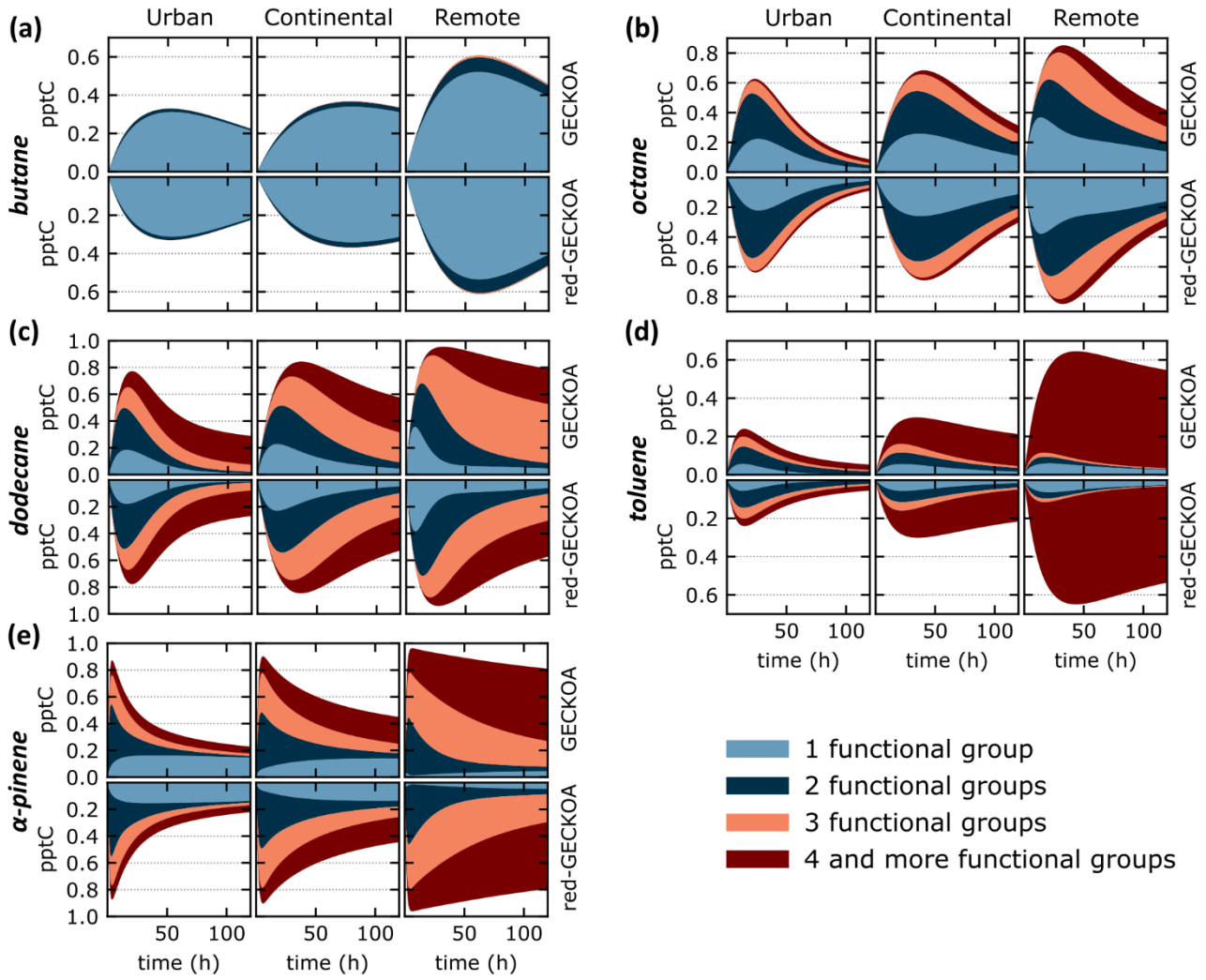


Figure S6: Temporal evolution of the mixing ratio (pptC) of secondary organic species summed across gas and particle phases and grouped by the number of functional groups on the carbon backbone for various parent hydrocarbons under different environmental scenarios. Panels (a–e): butane, octane, dodecane, toluene, and α-pinene as parent hydrocarbons, respectively. From left to right in each panel: urban, continental, and remote scenarios. Top and bottom rows in each panel: GECKO-A and red-GECKO-A simulation results, respectively. The color indicates the number of functional groups borne by the carbon backbone of each species.

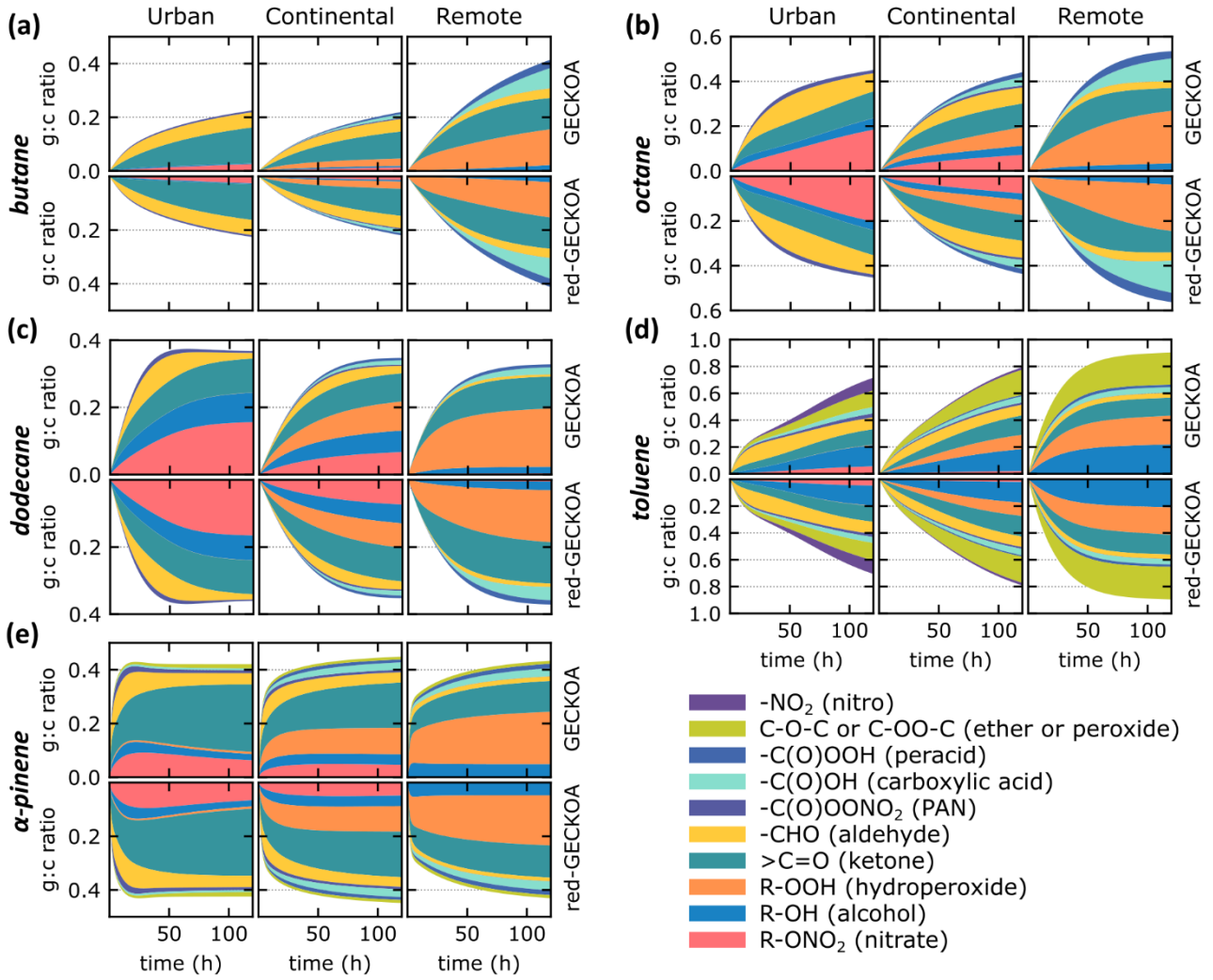


Figure S7: Temporal evolution of the functional group to carbon ratio $r_{g:c}$ for various parent hydrocarbons under different environmental scenarios. Panels (a–e) correspond to butane, octane, dodecane, toluene, and α-pinene, respectively. From left to right in each panel: urban, continental, and remote scenarios. The top and bottom rows show results from GECKO-A and red-GECKO-A simulations, respectively. Colors indicate the contribution of each organic functional group to the overall degree of organic carbon functionalization assessed across gas and particle phases.

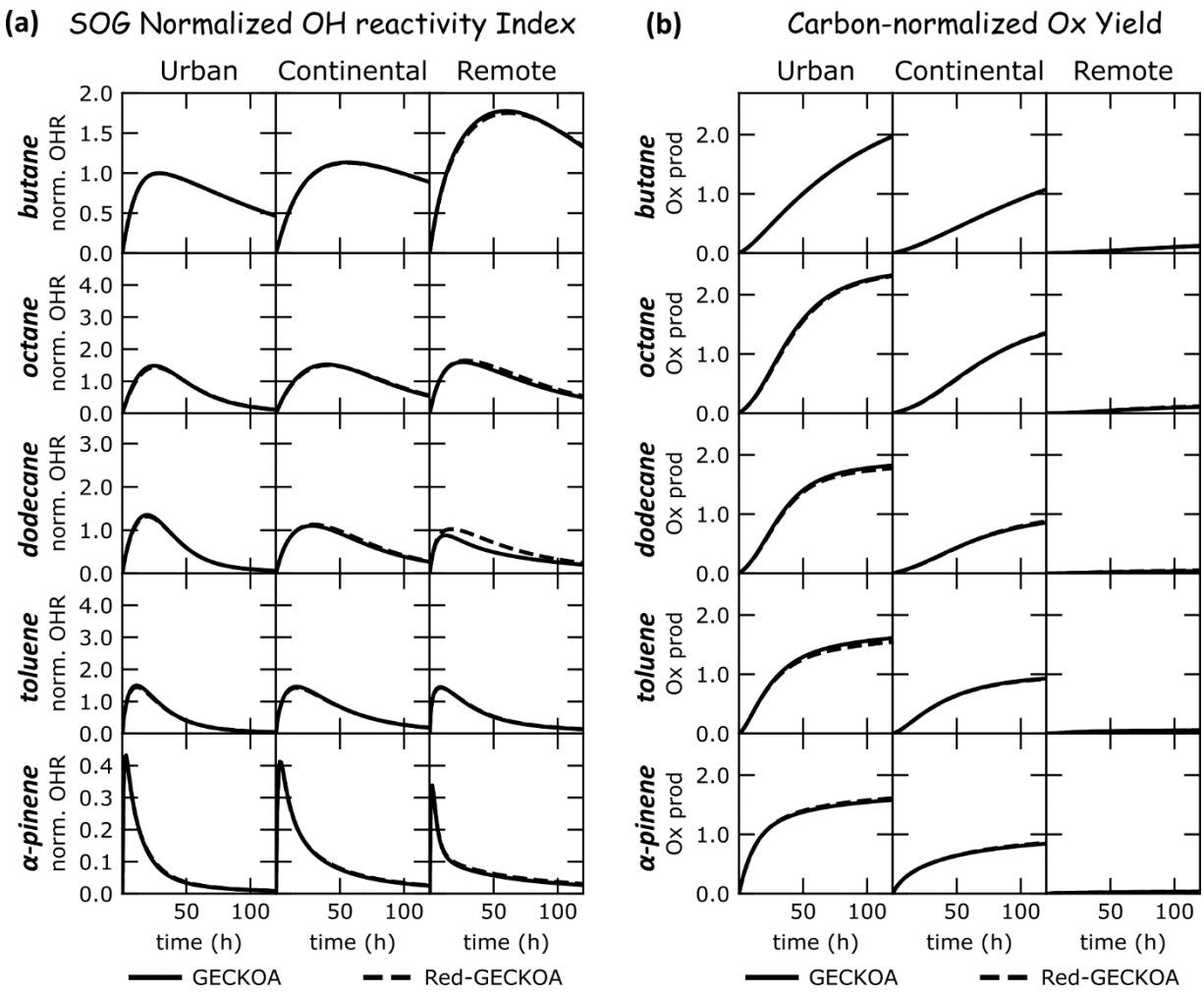


Figure S8: Temporal evolution of the SOG normalized OH reactivity index (panel a) and the carbon-normalized O_x yield (panel b) for various parent hydrocarbons under different environmental scenarios. From left to right: urban, continental, and remote scenarios. From top to bottom: butane, octane, dodecane, toluene, and α-pinene as parent compounds. Solid lines: GECKO-A simulation results; dashed lines: red-GECKO-A simulation results.

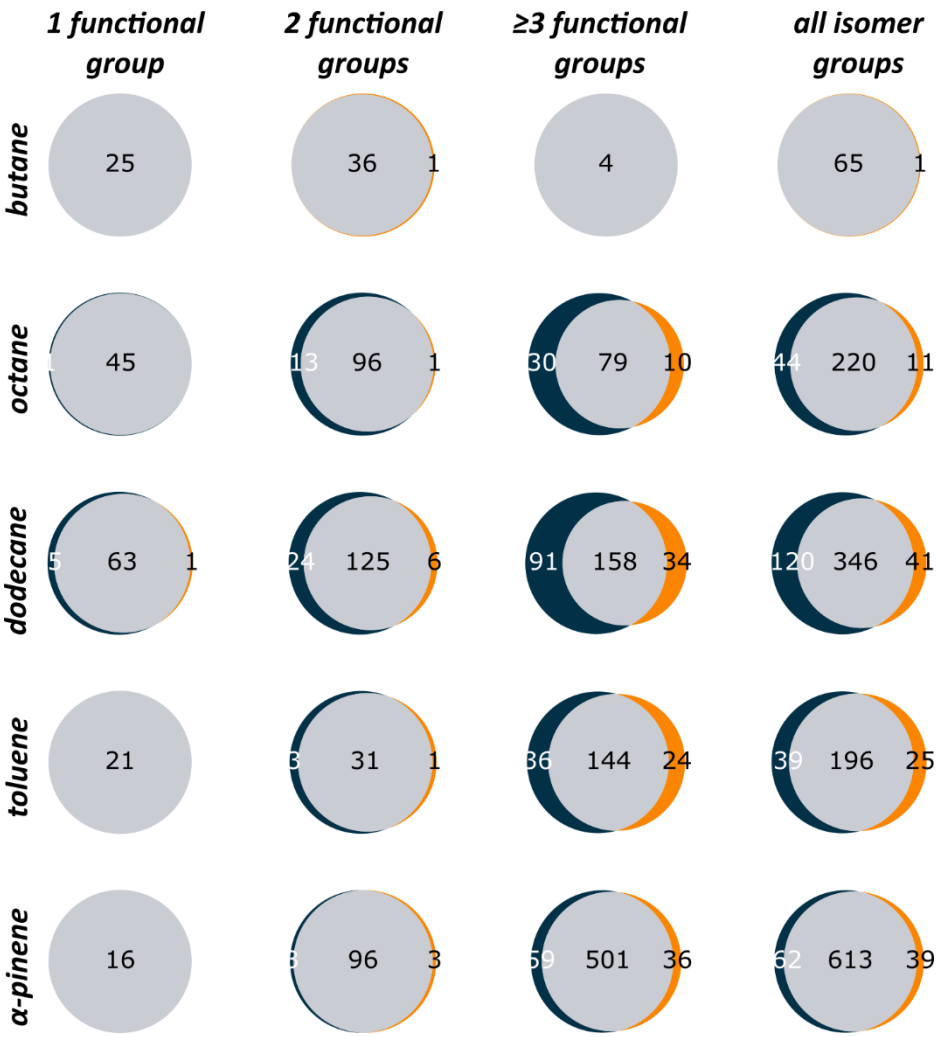


Figure S9: Number of non-radical isomer groups contributing to the carbon budget in the continental scenario, partitioned by presence in GECKO-A only, red-GECKO-A only, or both mechanisms. Left to right panels: monofunctional isomers, bifunctional isomers, polyfunctional isomers (more than two functional groups) and all isomer groups. Top to bottom panels: butane, octane, dodecane, toluene, and α-pinene as parent compounds. Blue: isomer groups present only in GECKO-A; orange: isomer groups present only in red-GECKO-A; gray: isomer groups common to both mechanisms.

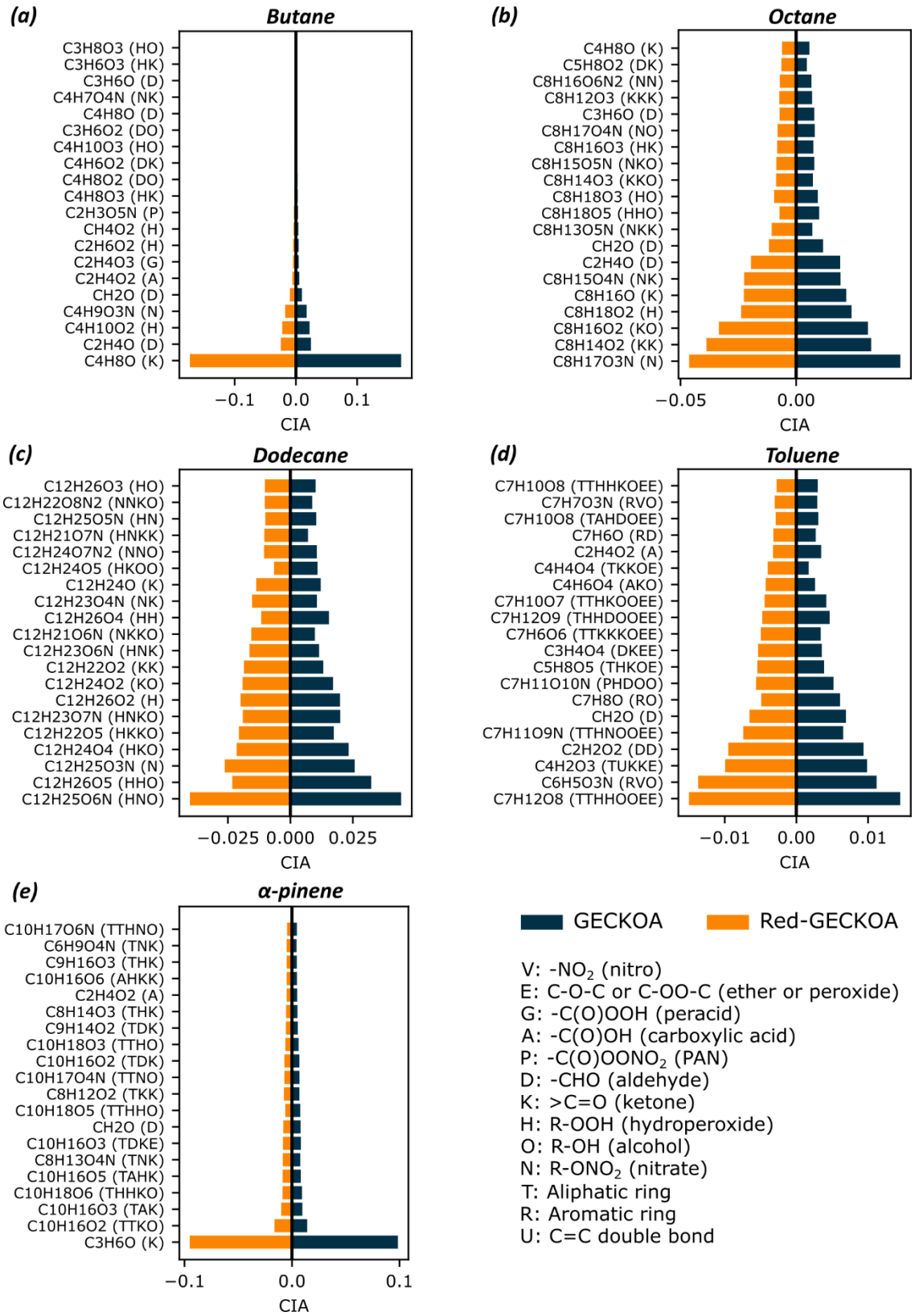


Figure S10: Major isomer groups contributing to the all-phases carbon budget in the continental scenario. Panels (a–e) correspond to butane, octane, dodecane, toluene, and α-pinene, respectively. Isomer groups are ranked by decreasing carbon-integrated abundance (CIA, see text) without mechanism distinction. Labels report the molecular formula of each group, and codes in parentheses indicate the functional groups on the carbon skeleton as specified in the legend. Left bars (orange): red-GECKO-A; right bars (blue): GECKO-A.

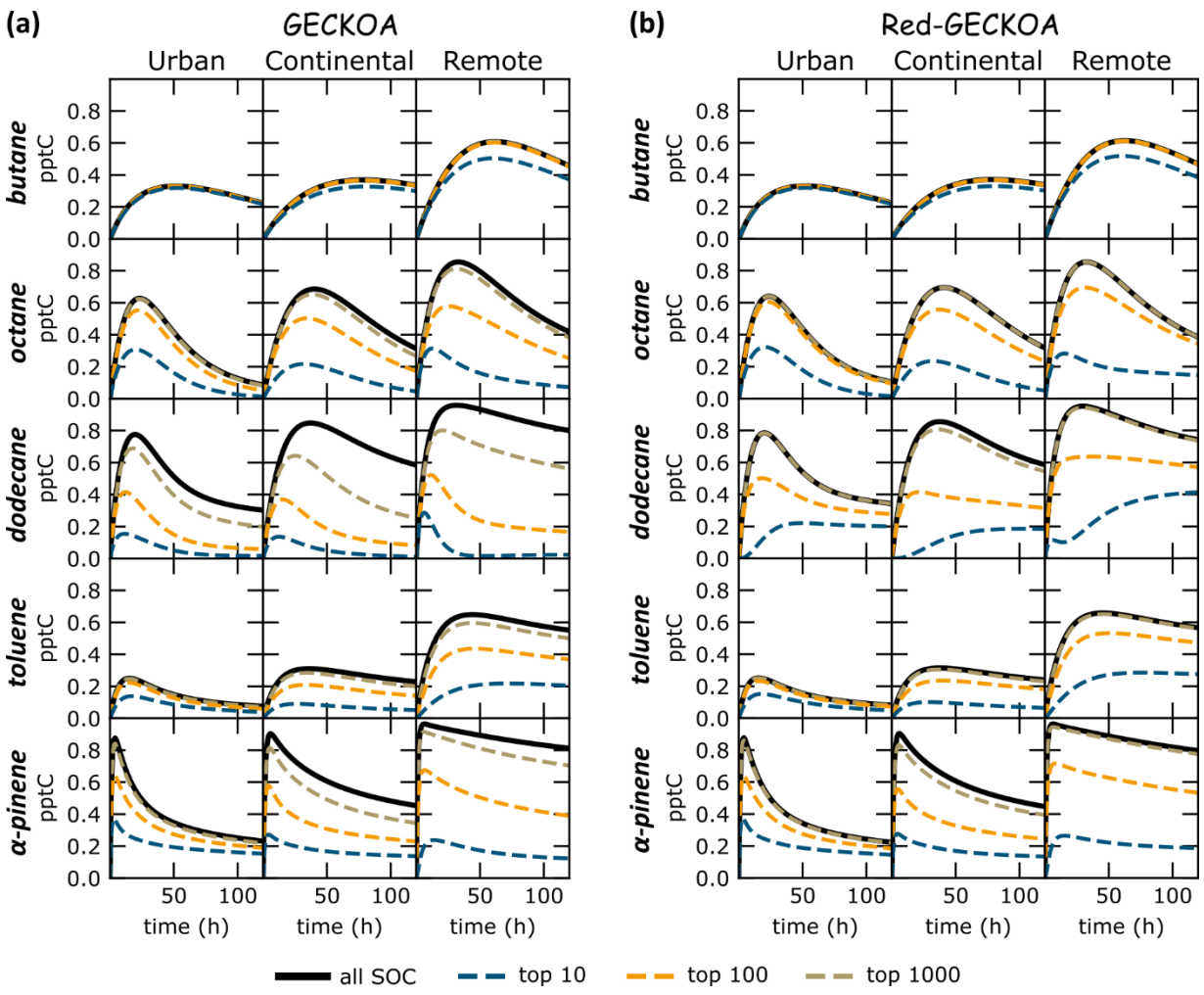


Figure S11: Temporal evolution of cumulative secondary organic carbon (SOC) contributions in GECKO-A (panel a) and red-GECKO-A (panel b) simulations for various parent hydrocarbons under different environmental scenarios. Columns (left to right): urban, continental, and remote scenarios. Rows (top to bottom): butane, octane, dodecane, toluene, and α-pinene as parent compounds. Black solid lines: total SOC; blue dashed lines: cumulative contribution of the top 10 species by carbon-integrated abundance; orange dotted lines: top 100 species; gray dotted lines: top 1000 species.

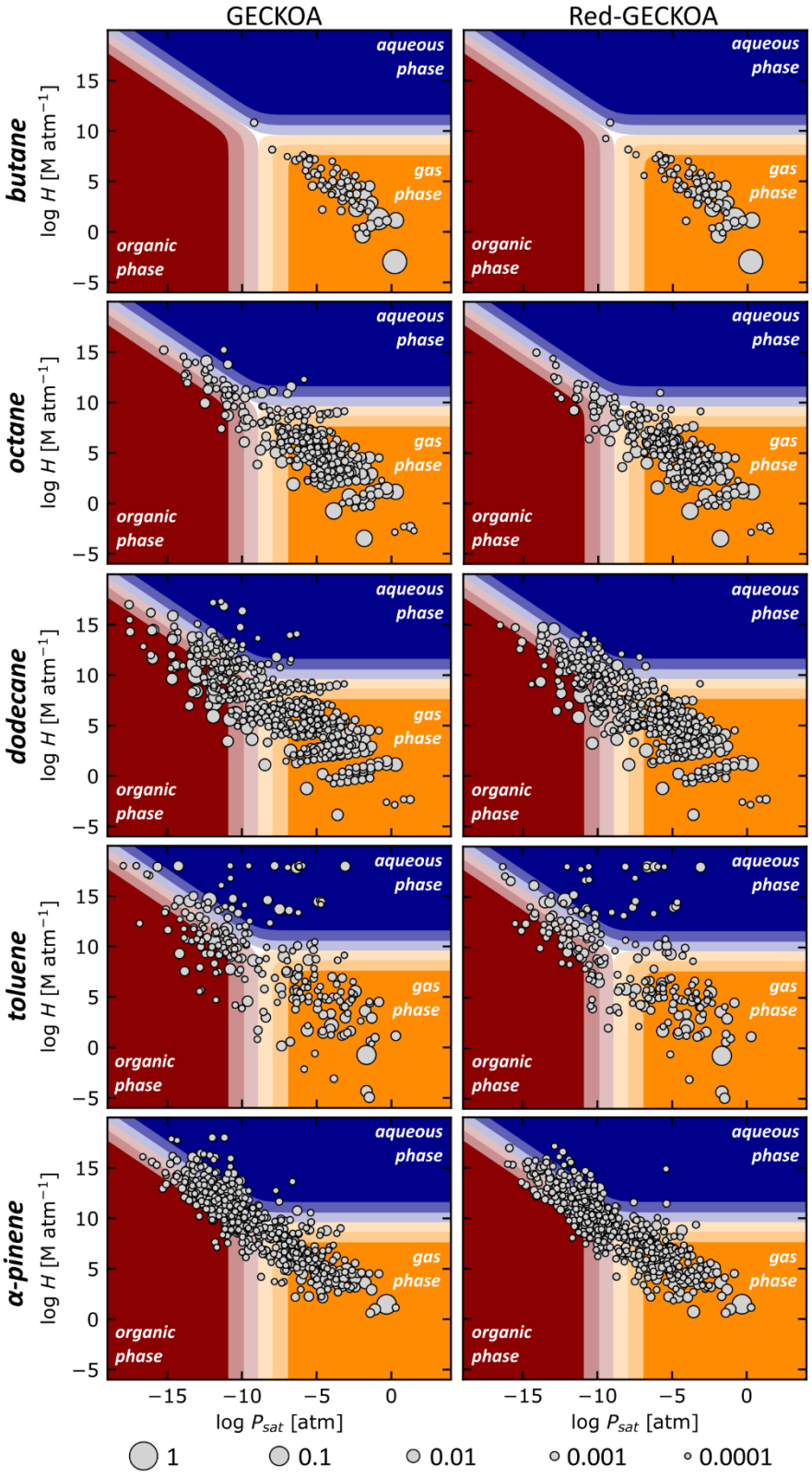


Figure S12: Distribution of species from GECKO-A (left column) and red-GECKO-A (right column) as a function of their saturation vapor pressure and effective Henry's law constant, for the continental scenario after 72 hours of simulation. From top to bottom: butane, octane, dodecane, toluene, and α-pinene as parent compounds. Colored domains indicate the dominant phase of each species at thermodynamic equilibrium: dark, intermediate, and light shades representing partitioning greater than 99%, 90%, and 50% in the respective phase. Domain boundaries are calculated for a mass concentration of 10 µg m^{-3} in both organic particulate and aqueous phases. Bubble size represents the relative carbon abundance of each species normalized to the initial parent compound.