Desorption Lifetimes and Activation Energies Influencing Gas-Surface Interactions and Multiphase Chemical Kinetics

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This Supplement comprises of seven figures (S1-S7).
Figure S1. The temperature dependence of the Henry’s law coefficient is shown using the van’t Hoff equation with solvation enthalpy of 20 kJ mol\(^{-1}\).
Figure S2. Coefficients derived from principal component analysis to examine the dependencies between the desorption energy ($E_{\text{des}}^0$), polarizability (polar, $\alpha$), dipole moment (dipole, $\mu$), oxygen to carbon ratio ($O:C$), and relative permittivity of the substrates (dielectric, $\varepsilon_r$).
Figure S3. Desorption energy \(E_{\text{des}}^0\) as a function of gas species polarizability \(\alpha\) in panel (a) and as a function of oxidation state of gas species expressed as \(O:C\) (b) using data from Tables A1-A15. Panels (a) and (b) reflect data from Fig. 8.
Figure S4. $E^0_{\text{des}}$ values derived from the new parameterization (Eq. (16)) applying arbitrary values of molar mass ($M$) and $O: C$, the latter coded as symbol color described by the color bar.
Figure S5. The dipole moment ($\mu$) is plotted against the polarizability ($\alpha$) where color shading indicates the oxidation state ($O:C$). Note that three gas species with $O:C > 1$ (CO$_2$ and formic acid) are included in this plot as having $O:C = 1$ to allow for better visualization of entire data set.
Figure S6. Calculated desorption energies ($E_{\text{des}}^0$) of SOA precursor gases from (Shiraiwa et al., 2014) as a function molar mass and its dependence on $O:C$ (a) and polarizability (b) using parameterization Eq. (16).
Figure S7. Relationship between calculated desorption energies ($E_{\text{des}}^0$) of SOA precursor gases from (Shiraiwa et al., 2014) and species’ glass transition temperature ($T_g$) and its dependence on $O:C$ (a) and molar mass (b) using parameterization Eq. (16).
References