

Estimation of liquid water content of tubing

To estimate the liquid water content of tubing necessary to produce the delays presented in Figure 6, the chromatographic model of Pagonis et al. (2017) was adapted to estimate total tubing surface water present (W , in mL m^{-2}) in place of effective absorbing wall mass (C_w). Instead of the gas-wall equilibrium constant (K_{gw}) in the model being determined by the analyte's saturation vapor concentration (C^*) and C_w , the equilibrium constant was calculated using the analyte's Henry's Law coefficient (H) and W :

$$K_{gw} = \frac{C_w}{C^*} \quad (1)$$

$$K_{gw} = A \frac{W}{H} \quad (2)$$

where A is a term that includes the surface area of the tube and the necessary terms of the ideal gas law to express K_{gw} in terms of moles of analyte dissolved in surface water per mole of gas-phase analyte in the tube. All other aspects of the tubing model were the same as those published in Pagonis et al. (2017).

Table S1. The semi- and low volatility compounds measured in this study. Products are grouped by compound and classified as the following: HN=hydroxynitrate, DHN=dihydroxynitrate, and
15 DHC=dihydroxycarbonyl.

Compound				SIMPOL C^*
Class	Formula	MW	Precursor	($\mu\text{g m}^{-3}$)
HN	$\text{C}_6\text{H}_{13}\text{NO}_4$	163	Hexanol	3.56E+04
HN	$\text{C}_8\text{H}_{17}\text{NO}_4$	191	Octanol	5.49E+03
HN	$\text{C}_9\text{H}_{19}\text{NO}_4$	205	Nonanol	2.14E+03
HN	$\text{C}_{10}\text{H}_{21}\text{NO}_4$	219	Decanol	8.30E+02
HN	$\text{C}_{12}\text{H}_{25}\text{NO}_4$	247	Dodecanol	1.23E+02
DHN	$\text{C}_6\text{H}_{13}\text{NO}_5$	179	Hexanol	2.46E+02
DHN	$\text{C}_8\text{H}_{17}\text{NO}_5$	207	Octanol	3.76E+01
DHN	$\text{C}_9\text{H}_{19}\text{NO}_5$	221	Nonanol	1.46E+01
DHN	$\text{C}_{10}\text{H}_{21}\text{NO}_5$	235	Decanol	5.57E+00
DHN	$\text{C}_{12}\text{H}_{25}\text{NO}_5$	263	Dodecanol	8.29E-01
DHC	$\text{C}_8\text{H}_{16}\text{O}_3$	160	Octanol	5.09E+02
DHC	$\text{C}_9\text{H}_{18}\text{O}_3$	174	Nonanol	2.02E+02
DHC	$\text{C}_{10}\text{H}_{20}\text{O}_3$	188	Decanol	7.96E+01
DHC	$\text{C}_{12}\text{H}_{24}\text{O}_3$	216	Dodecanol	1.22E+01

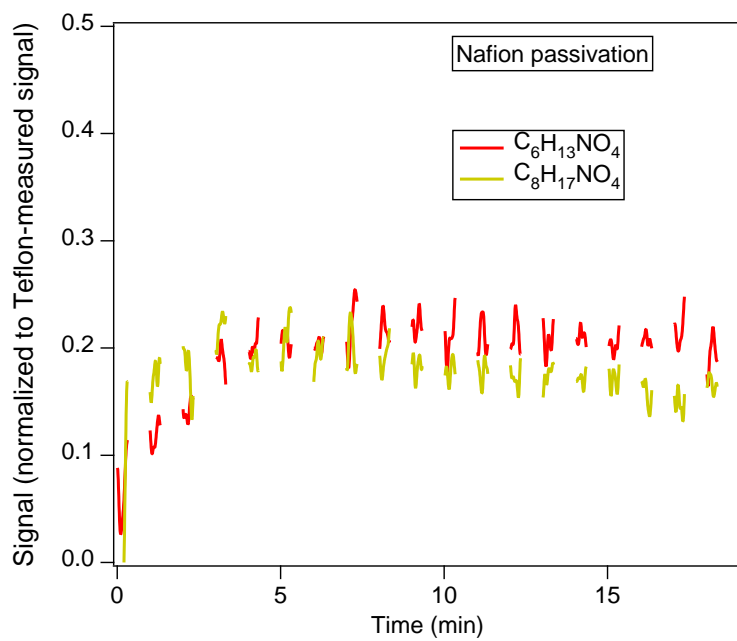


Figure S1. Passivation examples of Nafion tubing.

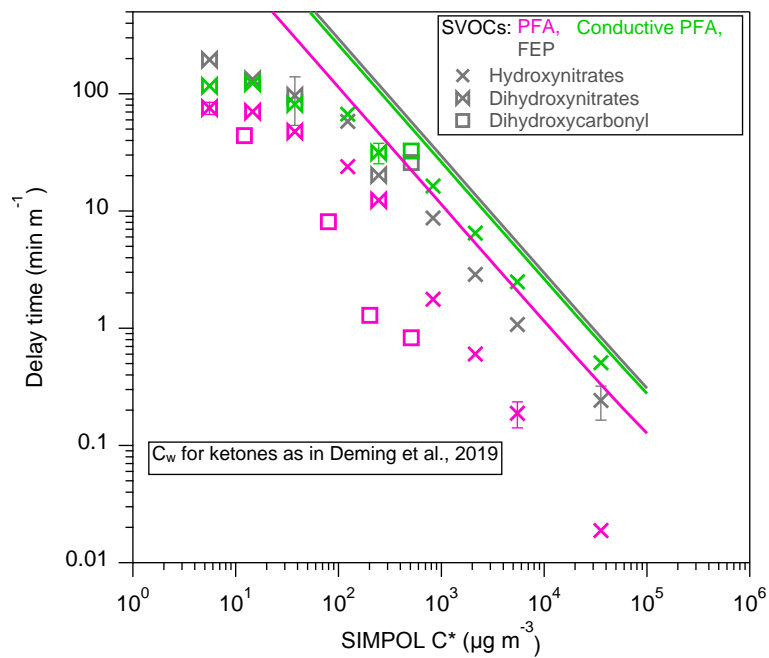


Figure S2. Modeled delays for volatility range studied in this work using the C_w estimated for ketones in Deming et al. (2019) at the same flow rate as measured.

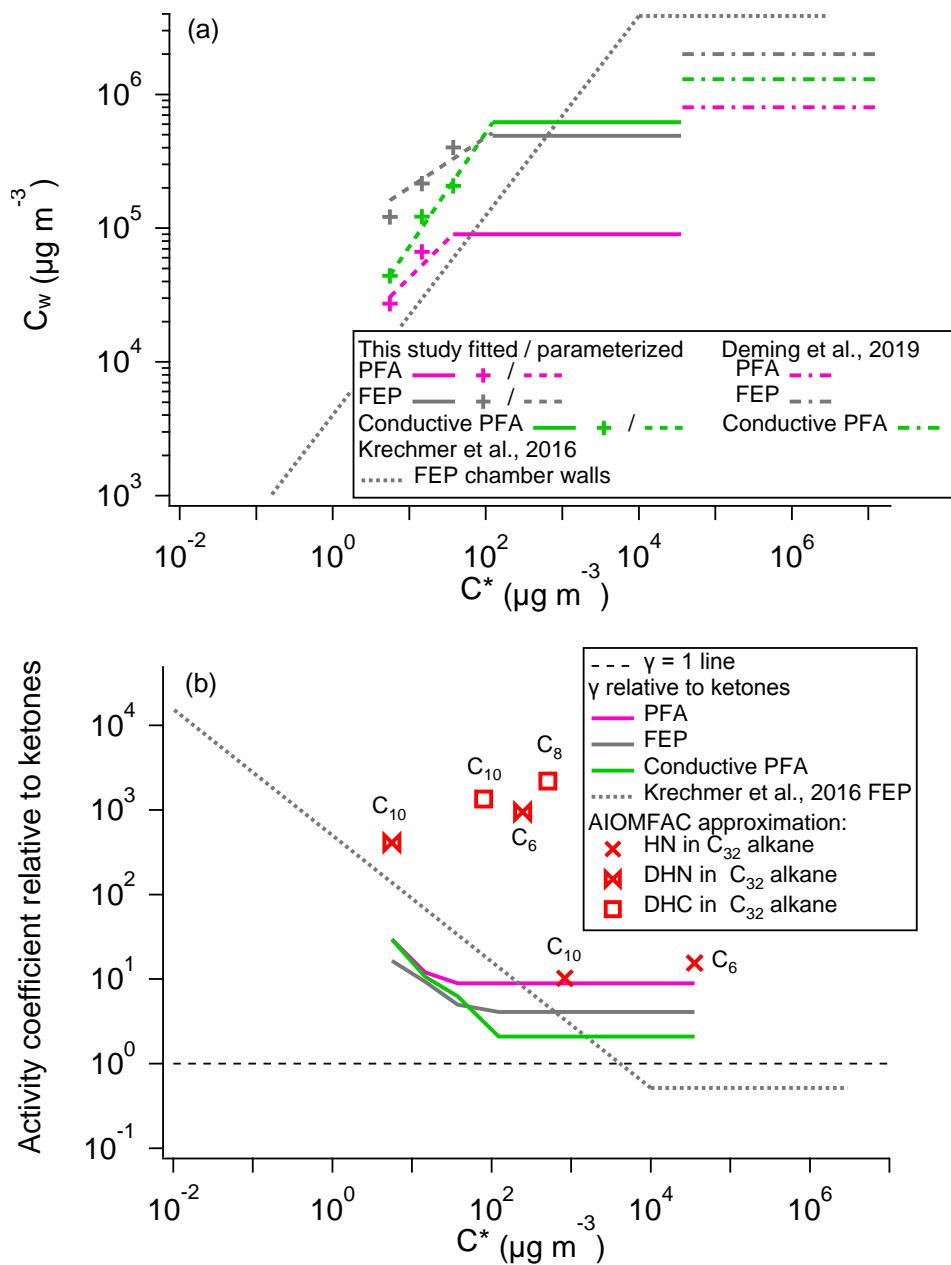


Figure S3. (a) Fitted values of C_w ($\mu\text{g m}^{-3}$) using the model for S/IVOCs into Teflon tubing materials (Table 2) and previously reported values from Deming et al. (2019) for tubing and Krechmer et al. (2016) for an FEP bag as a function of C^* . The solid lines and points represent C_w obtained from the model for C^* ranges $10^2 - 10^4$ and $5-10^2 \mu\text{g m}^{-3}$, respectively. The dashed lines were calculated using the

parameterization equations for C^* between $5\text{-}10^2 \mu\text{g m}^{-3}$ in Table 2. The Krechmer et al. (2016) line has been adjusted to tubing S/V ratio and same partitioning depth in FEP sheet and tubing is assumed. (b)
40 Relative activity coefficient γ of S/IVOCS to those of ketones partitioned in each tubing material (Deming et al., 2019). Also shown are AIOMFAC (Zuend et al., 2011) estimated γ (relative to 2-tetradecanone, the least volatile ketone used by Deming et al. (2019) for several species in long chain alkane, which mimics non-polar Teflon polymers. Note that the addition of an extra OH functional group can increase γ by over an order of magnitude.

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References

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