

Supporting information for:

Atmospheric degradation of cyclic volatile methyl siloxanes: Radical chemistry and oxidation products

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1. Peak-fitting of HR-CIMS data

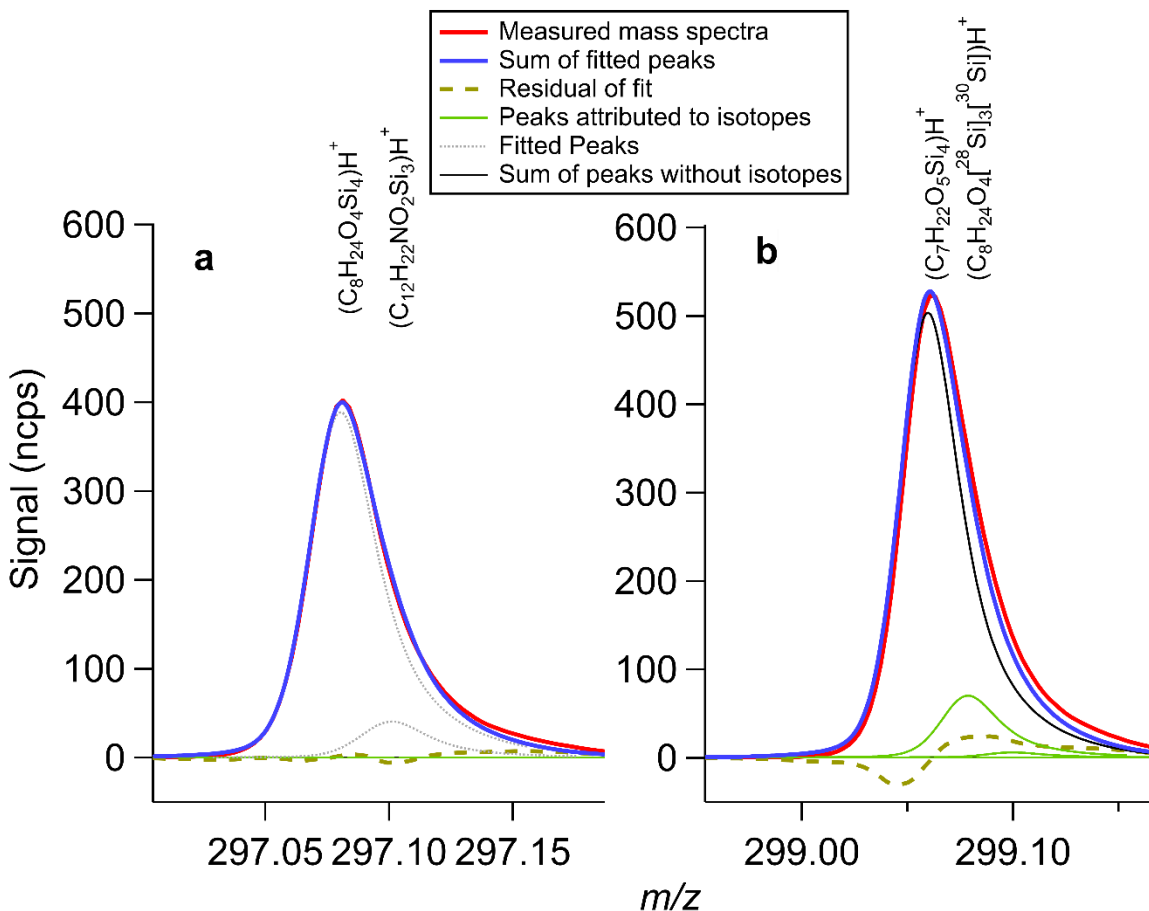


Figure S1 Example of the peak fitting and isotopic allocations for (a) D4 and (b) siloxanol product which overlaps with the D4 isotope signal, performed in Tofware. Isotopes and fitted peaks are labeled with their formulas.

All analysis of the chemical ionization mass spectrometer data was performed in Tofware v3.2.3 within the IgorPro v8.0.4.2 environment. As there is no separation technique of the oxidation products before entering the mass spectrometer, we need to consider potential overlap from the stable isotopes of the parent species with their oxidation products. For instance, an isotope of D4, $C_8H_{24}O_4[^{28}Si]_2[^{29}Si]_2$ (298.074 amu) and the siloxanol $C_7H_{22}O_5[^{28}Si]_4$ (298.054 amu) are only different by 0.02 amu (not shown in Figure S1). The mass spectrometer has a resolving power of $\sim 8000 \Delta m/z/m/z$. While this is insufficient for baseline resolution between peaks of interest at the same nominal mass, once we define the shapes of the peaks in Tofware, we can use fully

constrained peak fitting after subtracting constrained isotopic signal to best fit the peaks corresponding to different ions, even if they are significantly overlapping.

2. KinSim mechanism and kinetic inputs

The KinSim cases in IGOR Pro format used in this publication are available upon request. The model simulated ambient conditions (860 mbar and 25°C). The reactions and rate constants for the inorganic reactions are in Table S1, the rate constants for oxidation with OH and Cl in addition to reactions with NO and HO₂ are in Table S2. The different isomerization reactions are listed in Table S3 and the reactions used to calculate wall partitioning are in Table S4. Explanations of the names are in Table S5.

Table S1 Non-cVMS reactions used in the KinSim mechanism

Reactant 1	Reactant 2	Product 1	Product 2	Product 3	<i>k</i>
H2O2	hv	OH	OH		7.0×10^{-5}
Cl2	hv	Cl	Cl		2.0×10^{-4}
HONO	hv	OH	NO		3.0×10^{-4}
O3	hv	O1D	O2		5.0×10^{-5}
NO2	hv	NO	O1D		3.0×10^{-7}
HO2	hv	OH	O1D		1.0×10^{-9}
O1D	H2O	OH	OH		2.0×10^{-10}
O1D	N2	O3P	N2		2.6×10^{-11}
OH	H2O2	HO2	H2O		1.7×10^{-12}
OH	NO	HNO2			3.3×10^{-11}
OH	HNO3	H2O	NO2		1.5×10^{-13}
HO2	NO2	HNO4			4.7×10^{-12}
NO2	NO3	N2O5			1.9×10^{-12}
N2O5		NO2	NO3		7.0×10^{-2}
O3P	O2	O3			2.8×10^{-12}
O3P	NO	NO2			3.0×10^{-11}
CH2O	Cl	HO2	CO		7.3×10^{-11}
CO	OH	CO2	H		1.5×10^{-13}
CO	O1D	CO2			8.0×10^{-11}
H	OH	H2O			2.5×10^{-10}
H	Cl	HCl			2.5×10^{-10}
CO	HO2	CO2	OH		1.0×10^{-17}
Cl	HO2	O2	HCl		3.4×10^{-11}
OH	HO2	H2O	O2		1.1×10^{-10}
Cl	CO	Sink			1.0×10^{-33}
HO2	HO2	H2O2	O2		4.0×10^{-12}
O3	OH	HO2			7.3×10^{-14}
HO2	O3	OH			2.0×10^{-15}

O1D	O2	O3P	O2		4.0×10^{-11}
O1D	O3	2 O2			1.2×10^{-10}
O1D	O3	O2	2 O1D		1.2×10^{-10}
O1D	OH	O2	H		4.0×10^{-11}
O1D	HO2	OH	O2		5.9×10^{-11}
O1D	H2O2	OH	HO2		1.7×10^{-15}
O1D	O3	2 O2			8.0×10^{-15}
H	O3	OH	O2		2.9×10^{-11}
HO2	NO	OH	NO2		8.7×10^{-12}
HO2	H	2 OH			7.2×10^{-11}
H	HO2	O1D	H2O		1.6×10^{-12}
H	HO2	O2	H2		6.9×10^{-12}
OH	H2	H2O	H		6.7×10^{-15}
OH	OH	H2O	O1D		1.8×10^{-12}
O1D	NO2	NO	O2		1.0×10^{-11}
O1D	NO2	NO3			2.0×10^{-11}
O1D	HO2NO2	NO2	H2O	O2	8.6×10^{-16}
H	NO2	OH	NO		1.3×10^{-10}
OH	NO3	HO2	NO2		2.2×10^{-11}
HO2	NO3	OH	NO2	O2	3.5×10^{-12}
NO	NO3	NO2	NO2		2.6×10^{-11}
NO3	NO3	2 NO2	O2		2.3×10^{-16}
HNO4		HO2	NO2		2.5×10^{-1}
N2O5	H2O	2 H2NO3			2.0×10^{-21}
NO	O3	NO2	O2		1.9×10^{-14}
NO2	O3	NO3	O2		3.2×10^{-17}
NO2	OH	HO2	NO		3.8×10^{-16}
OH	HNO4	NO2			4.7×10^{-12}
H	O2	HO2			6.0×10^{-32}
H	O2	OH	O1D		1.5×10^{-37}
CH2O	OH	HO2	CO		9.4×10^{-12}
CO	OH	CO2	HO2		1.5×10^{-13}

Table S2 Bimolecular reactions of Si-containing products.

Reactant 1	Reactant 2	Product 1	Product 2	Product 3	k
D3 ^a	OH	D3CH2OO	H2O		8.6×10^{-13}
D3	Cl	D3CH2OO	HCl		5.6×10^{-11}
D4	OH	D4CH2OO	H2O		1.3×10^{-12}
D4	Cl	D4CH2OO	HCl		1.2×10^{-10}
D5	OH	D5CH2OO	H2O		2.1×10^{-12}
D5	Cl	D5CH2OO	HCl		1.8×10^{-10}
D3OH	OH	D3OHCH2OO	H2O		8.6×10^{-13}
D3OH	Cl	D3OHCH2OO	HCl		5.6×10^{-11}
D4OH	OH	D4OHCH2OO	H2O		1.3×10^{-12}
D4OH	Cl	D4OHCH2OO	HCl		1.2×10^{-10}
D5OH	OH	D5OHCH2OO	H2O		2.1×10^{-12}
D5OH	Cl	D5OHCH2OO	HCl		1.8×10^{-10}
D3FormEst	OH	D3FormEstCH2OO	H2O		8.6×10^{-13}
D3FormEst	Cl	D3FormEstCH2OO	HCl		5.6×10^{-11}
D4FormEst	OH	D4FormEstCH2OO	H2O		1.3×10^{-12}
D4FormEst	Cl	D4FormEstCH2OO	HCl		1.2×10^{-10}
D5FormEst	OH	D5FormEstCH2OO	H2O		2.1×10^{-12}
D5FormEst	Cl	D5FormEstCH2OO	HCl		1.8×10^{-10}
D3(OH)2	OH	Sink ^b	H2O		8.6×10^{-13}
D3(OH)2	Cl	Sink	HCl		5.6×10^{-11}
D4(OH)2	OH	Sink	H2O		1.3×10^{-12}
D4(OH)2	Cl	Sink	HCl		1.2×10^{-10}
D5(OH)2	OH	Sink	H2O		2.1×10^{-12}
D5(OH)2	Cl	Sink	HCl		1.8×10^{-10}
D3(FormEst)2	OH	Sink	H2O		8.6×10^{-13}
D3(FormEst)2	Cl	Sink	HCl		5.6×10^{-11}
D4(FormEst)2	OH	Sink	H2O		1.3×10^{-12}
D4(FormEst)2	Cl	Sink	HCl		1.2×10^{-10}
D5(FormEst)2	OH	Sink	H2O		2.1×10^{-12}
D5(FormEst)2	Cl	Sink	HCl		1.8×10^{-10}
D3OHFormEst	OH	Sink	H2O		8.6×10^{-13}
D3OHFormEst	Cl	Sink	HCl		5.6×10^{-11}
D4OHFormEst	OH	Sink	H2O		1.3×10^{-12}
D4OHFormEst	Cl	Sink	HCl		1.2×10^{-10}
D5OHFormEst	OH	Sink	H2O		2.1×10^{-12}
D5OHFormEst	Cl	Sink	HCl		1.8×10^{-10}
D3CH2OO ^c	HO2	0.9 D3CH2O	0.9 OH	0.1 D3CH2OOH	1.7×10^{-11}
D3CH2OO ^c	NO	D3CH2O	NO2		9.0×10^{-12}
D3O ^d	H2O	D3OH	OH		5.0×10^{-15}
D3O	HO2	D3OH	O2		1.7×10^{-11}

^aReactions of the closed-shell oxidation products had the same rate constants as the parent cVMS. ^bTas we were focused on the first-generation products, once a cVMA had two methyl groups replaced and was oxidized, it was no longer considered. ^cThe rate constants and branching ratios of reactions between RO₂ with HO₂, NO, and other RO₂ radicals was kept constant for all cVMS and their oxidation products. ^dThe rate constant of reactions between RO and H₂O as well as for the addition of O₂ to the alkyl radicals were also kept constant.

Table S3 Unimolecular/pseudo-unimolecular reactions rate constants of Si-containing products.

Reactant 1	Product 1	Product 2	k
D3CH2OO	D3O	CH2O	8.0×10^{-3}
D3CH2O	D3OCH2		1.0×10^{10}
D3OCH2O	D3FormEst	HO2	1.0×10^4
D3OHO	Sink		1.1×10^3
D3OHCH2OO	D3OHO	CH2O	9.0×10^{-1}
D3OHCH2O	D3OHOCH2		1.0×10^9
D3OHOCH2O	D3OHFormEst	HO2	1.0×10^4
D3FormEstCH2OO	D3FormEstO	CH2O	9.0×10^{-1}
D3FormEstO	Sink		1.1×10^3
D3FormEstCH2O	D3FormEstOCH2		1.0×10^9
D3FormEstOCH2	D3FormEstOCH2OO		1.0×10^{11}
D3FormEstOCH2O	D3FormEst2	HO2	1.0×10^4
D3O	D3OHCH2OO		1.1×10^3
D4CH2OO	D4O	CH2O	8.0×10^{-3}
D4CH2O	D4OCH2		1.0×10^9
D4OCH2O	D4FormEst	HO2	1.0×10^4
D4OHCH2OO	D4OHO	CH2O	9.0×10^{-1}
D4OHO	Sink		5.1×10^3
D4OHCH2O	D4OHOCH2		1.0×10^9
D4OHOCH2O	D4OHFormEst	HO2	1.0×10^4
D4FormEstCH2OO	D4FormEstO	CH2O	9.0×10^{-1}
D4FormEstO	Sink		5.1×10^3
D4FormEstCH2O	D4FormEstOCH2		1.0×10^9
D4FormEstOCH2O	D4FormEst2	HO2	1.0×10^4
D4O	D4OHCH2OO		1.1×10^3
D5CH2OO	D5O	CH2O	8.0×10^{-3}
D5CH2O	D5OCH2		1.0×10^9
D5OCH2O	D5FormEst	HO2	1.0×10^4
D5OHCH2OO	D5OHO	CH2O	9.0×10^{-1}
D5OHO	Sink		5.1×10^3
D5OHCH2O	D5OHOCH2		1.0×10^9
D5OHOCH2	D5OHOCH2OO		1.0×10^{11}
D5FormEstO	Sink		5.1×10^3
D5FormEstCH2OO	D5FormEstO	CH2O	9.0×10^{-1}
D5FormEstCH2O	D5FormEstOCH2		1.0×10^9
D5FormEstOCH2O	D5FormEst2	HO2	1.0×10^4
D5O	D5OHCH2OO		1.1×10^3

Table S4 Inputs used to calculate wall partitioning in the model

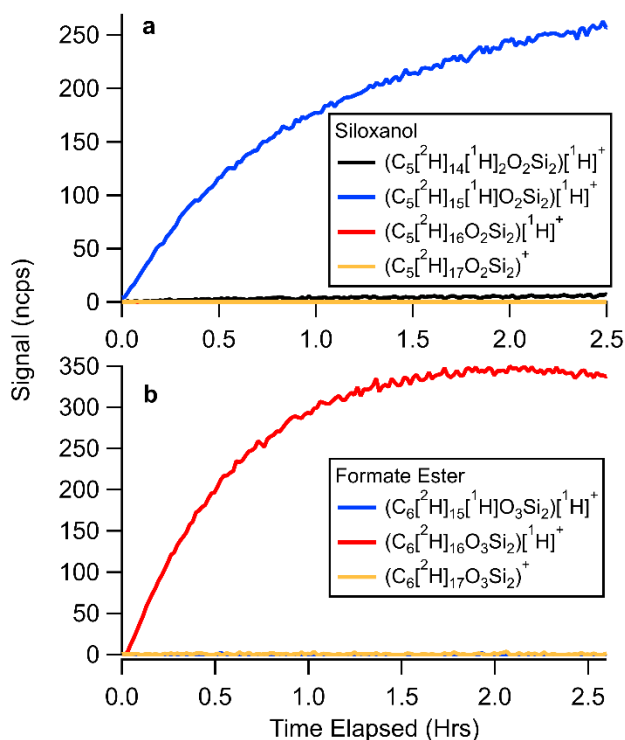
Reactant 1	Product 1	A Ainf	E Einf	N ninf
D3	w_D3	4.39×10^7	4.00×10^3	1×10^{-3}
w_D3	D3	4.39×10^7	0	1×10^{-3}
D3FormEst	w_D3FormEst	2.83×10^7	4.60×10^3	1×10^{-3}
w_D3FormEst	D3FormEst	2.83×10^7	0	1×10^{-3}
D3FormEst2	w_D3FormEst2	1.27×10^7	4.83×10^3	1×10^{-3}
w_D3FormEst2	D3FormEst2	1.27×10^7	0	1×10^{-3}
D3OH	w_D3OH	1.82×10^6	4.88×10^3	1×10^{-3}
w_D3OH	D3OH	1.82×10^6	0	1×10^{-3}
D3OH2	w_D3OH2	8.20×10^3	5.64×10^2	1×10^{-3}
w_D3OH2	D3OH2	8.20×10^3	0	1×10^{-3}
D3OHFormEst	w_D3OHFormEst	6.05×10^4	5.40×10^3	1×10^{-3}
w_D3OHFormEst	D3OHFormEst	6.05×10^4	0	1×10^{-3}
D3OCH2OOH	w_D3OCH2OOH	8.41×10^5	5.26×10^3	1×10^{-3}
w_D3OCH2OOH	D3OCH2OOH	8.41×10^5	0	1×10^{-3}
D3CH2OOH	w_D3CH2OOH	2.95×10^6	5.03×10^3	1×10^{-3}
w_D3CH2OOH	D3CH2OOH	2.95×10^6	0	1×10^{-3}
D4	w_D4	2.10×10^7	4.52×10^3	1×10^{-3}
w_D4	D4	2.10×10^7	0	1×10^{-3}
D4FormEst	w_D4FormEst	3.75×10^6	5.09×10^3	1×10^{-3}
w_D4FormEst	D4FormEst	3.75×10^6	0	1×10^{-3}
D4FormEst2	w_D4FormEst2	2.16×10^6	5.29×10^3	1×10^{-3}
w_D4FormEst2	D4FormEst2	2.16×10^6	0	1×10^{-3}
D4OH	w_D4OH	1.54×10^5	5.33×10^3	1×10^{-3}
w_D4OH	D4OH	1.54×10^5	0	1×10^{-3}
D4OH2	w_D4OH2	9.08×10^2	6.02×10^3	1×10^{-3}
w_D4OH2	D4OH2	9.08×10^2	0	1×10^{-3}
D4OHFormEst	w_D4OHFormEst	7.16×10^3	5.81×10^3	1×10^{-3}
w_D4OHFormEst	D4OHFormEst	7.16×10^3	0	1×10^{-3}
D4OCH2OOH	w_D4OCH2OOH	1.35×10^5	5.68×10^3	1×10^{-3}
w_D4OCH2OOH	D4OCH2OOH	1.35×10^5	0	1×10^{-3}
D4CH2OOH	w_D4CH2OOH	4.45×10^5	5.68×10^3	1×10^{-3}
w_D4CH2OOH	D4CH2OOH	4.45×10^5	0	1×10^{-3}
D5	w_D5	4.86×10^6	4.96×10^3	1×10^{-3}
w_D5	D5	4.86×10^6	0	1×10^{-3}
D5FormEst	w_D5FormEst	7.74×10^5	5.47×10^3	1×10^{-3}
w_D5FormEst	D5FormEst	7.74×10^5	0	1×10^{-3}
D5FormEst2	w_D5FormEst2	4.80×10^5	5.66×10^3	1×10^{-3}
w_D5FormEst2	D5FormEst2	4.80×10^5	0	1×10^{-3}
D5OH	w_D5OH	2.69×10^4	5.71×10^3	1×10^{-3}
w_D5OH	D5OH	2.69×10^4	0	1×10^{-3}
D5OH2	w_D5OH2	1.94×10^2	6.33×10^3	1×10^{-3}
w_D5OH2	D5OH2	1.94×10^2	0	1×10^{-3}
D5OHFormEst	w_D5OHFormEst	1.13×10^3	6.14×10^3	1×10^{-3}
w_D5OHFormEst	D5OHFormEst	1.13×10^3	0	1×10^{-3}
D5OCH2OOH	w_D5OCH2OOH	2.95×10^4	6.02×10^3	1×10^{-3}
w_D5OCH2OOH	D5OCH2OOH	2.95×10^4	0	1×10^{-3}
D5CH2OOH	w_D5CH2OOH	9.23×10^4	5.83×10^3	1×10^{-3}
w_D5CH2OOH	D5CH2OOH	9.23×10^4	0	1×10^{-3}

Table S5 Abbreviations and meanings used in KinSim (shown for D5, but applies to all cVMS)

KinSim Name	Meaning
D5FormEst	D5 Formate Ester
D5OH	D5 Siloxanol
D5OH2	D5 Siloxandiol
D5FormEst2	D5 with Two Formate Ester Groups
D5CH2OOH	D5 Hydroperoxide
D5OCH2OOH	D5 Ether Hydroperoxide
D5OHCH2OO	D5 Siloxanol with an RO ₂

3. [²H]₁₈L2 oxidation with Cl atoms

In an experiment that is similar to one performed by Atkinson (1995)¹, fully deuterated hexamethyldisiloxane (D₁₈L2, or [²H]₁₈L2) was oxidized using Cl₂ as the oxidant precursor. The toluene used as the reagent ion was not isotopically labeled, so all charge-carrying species on the detected molecules will be ¹H. Trace water in the chamber was sufficient for labile hydrogen exchange. Figure S2 shows example time series of the products attributed to the siloxanol and the formate ester. The siloxanol has one

**Figure S2** Time series of the signals

corresponding to the (a) siloxanol and (b) formate ester products of [²H]₁₈L2. The trace colors are based on how many ¹H are present in the formula.

exchangeable H (aside from the charge carrying H) on the hydroxyl group. The other main product, $(C_6[{}^2H]_{16}O_3Si_2)[{}^1H]^+$, is only observed as the deuterated peak consistent with a formate ester rather than a carboxylic acid.

4. Assumptions and evidence for capturing most of the oxidation products

In Figure S4, the time-series of the sum of the products are shown versus the percentage of cVMS reacted. Although the total signals begin to diverge near the end of the experiments, at the point where 10% of the cVMS has been oxidized there is agreement within ~20% of the total product signal between the different conditions. As shown in Figure S3, the total signals vary minimally at the 10% cVMS reacted point between experiments, even when there are significant changes in the compositions of the ions formed (particularly for D3). Given the large changes in RO₂ fate between the different experimental conditions, we would expect to see larger deviations between experiments if we were failing to detect important oxidation products or if there were large variations in instrument response between the different compounds. Because of this, we expect that the different ions provide similar instrument responses to each other and that we are measuring most of the oxidation products.

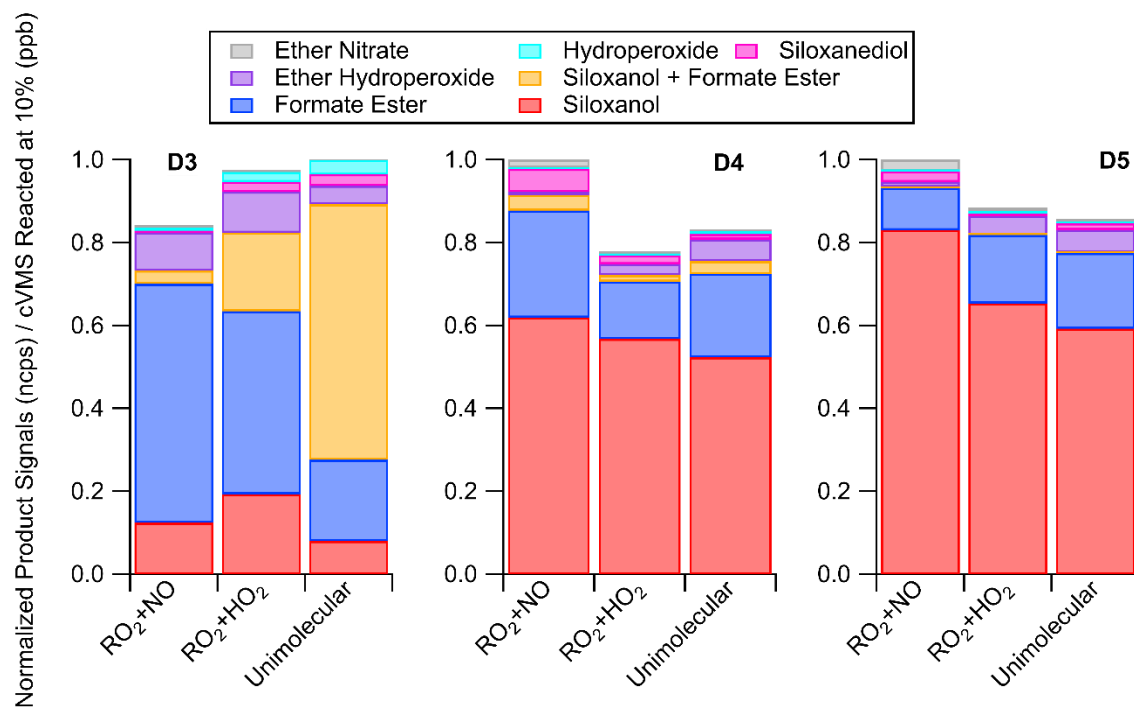


Figure S3 Sum of the product signals for the three cVMS investigated in all three conditions at the point where 10% of the cVMS was oxidized, normalized to the condition with the largest signal yield, colored by the identity of the signals.

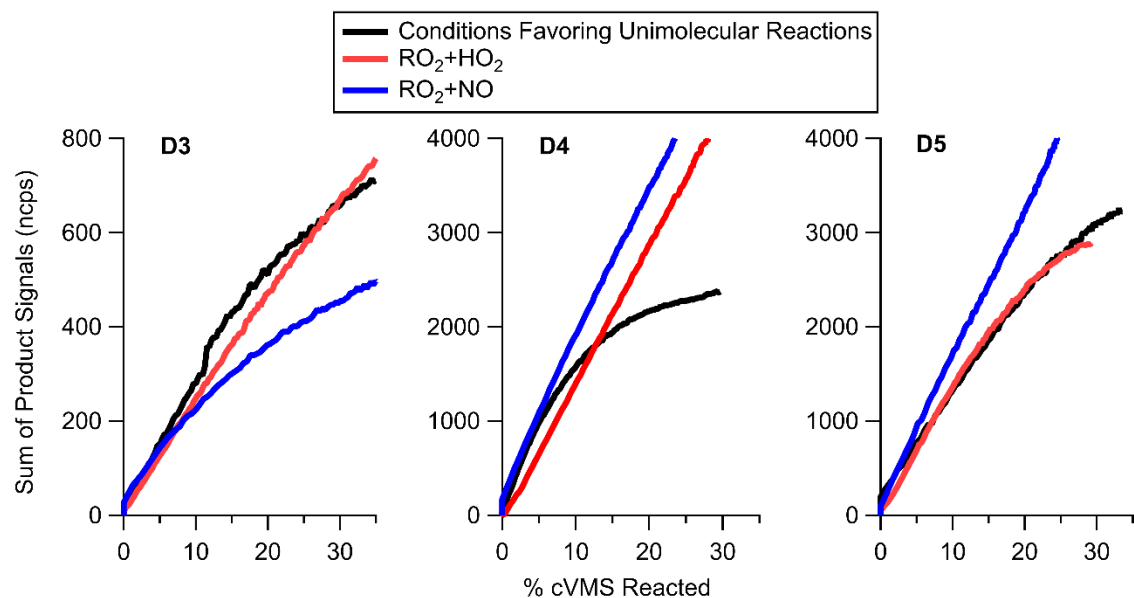


Figure S4 Sum of the product signals for the three different cVMS used plotted versus the percent of the parent cVMS lost.

5. Siloxanol Time-Series from Model and experiments

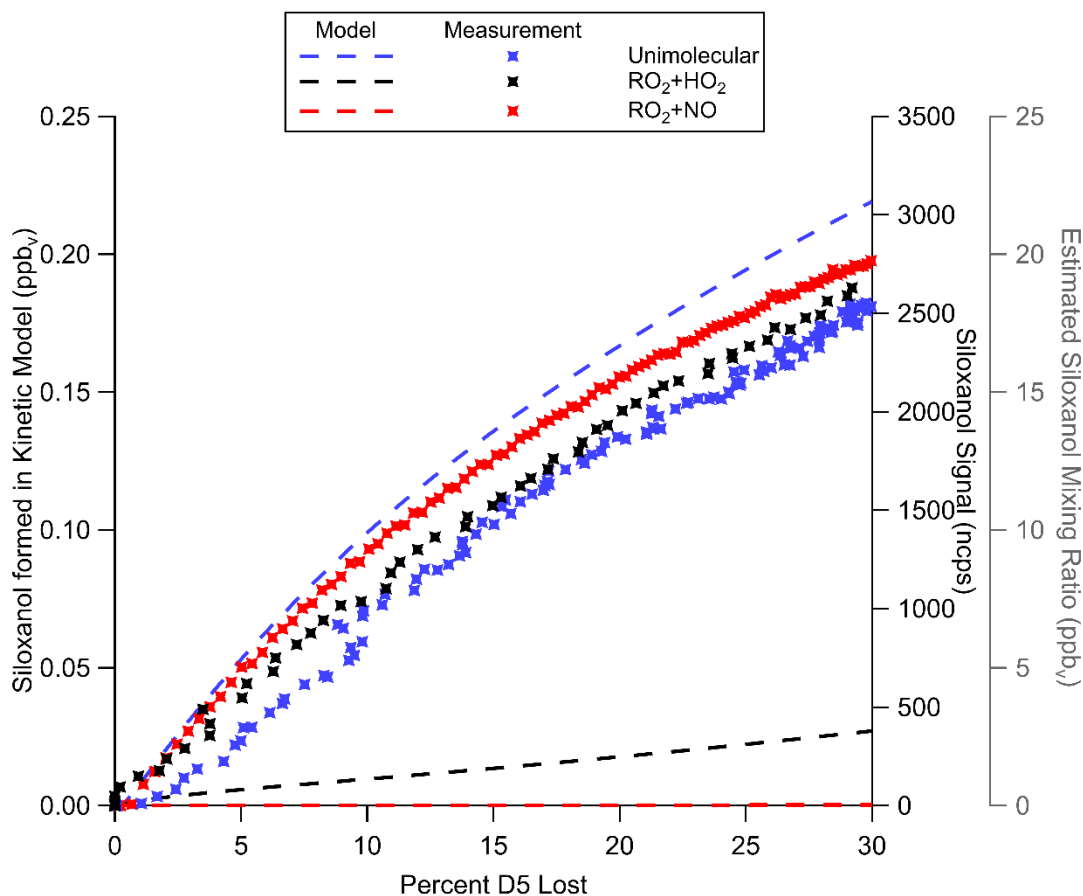


Figure S5 Time series of the siloxanol signals for D5 oxidation in our experiments (markers) and our kinetic model (dashed lines) plotted versus the percent of cVMS lost.

6. Estimated physical constants of cVMS oxidation products

Since there are no measurements of Henry's law constants for the oxidation products, we used three different methods to estimate the constants for the proposed products. Using EPIWEB v4.11, the vapor pressures/boiling points (MPBPWIN v1.44), water solubilities (WSKOW v1.43), and Henry's law constants (HENRY v3.21) were all calculated. No inputs were added aside from the structure of the product. Using the Toxicity Estimation Software Tool (TEST v5.1.1), the vapor pressures and water solubilities were calculated with the consensus method.

As a proxy for Henry's law, the ratio of vapor pressure to water solubility was also used, which is also reported in HENRY v3.21 using the water solubility estimate from WSKOW v1.43 and vapor pressure estimate from MPBPWIN v1.44. It is important to note that vapor pressure divided by water solubility is not equivalent to the Henry's Law constant. However, we are using this as an approximation to Henry's Law to compare between TEST and EPIWEB outputs. Table S6 contains the results of the three different methods.

Table S6: Estimated physical parameters of cVMS oxidation products for D3, D4, and D5 using both EPIWEB and TEST software.

Compound	Vapor Pressure (mmHg)		Water Solubility (log(mol L ⁻¹))		Henry's Solubility (M atm ⁻¹)	Vapor Pressure/Water Solubility (M atm ⁻¹)	
	MPBP	TEST	WSKOW	TEST	HENRYWin	HENRYWin	TEST
D3	3.49×10 ⁰	2.17×10 ⁰	-5.157	-6.14	6.45×10 ⁻⁴	1.61×10 ⁻³	2.54×10 ⁻⁴
D3OH	2.87×10 ⁻¹	1.10×10 ⁻¹	-2.991	-4.66	1.26×10 ⁺¹	2.70×10 ⁰	1.51×10 ⁻¹
D3 Formate Ester	1.87×10 ⁰	9.81×10 ⁻³	-4.096	-5.64	2.82×10 ⁻²	3.26×10 ⁻²	1.77×10 ⁻¹
D3OHFormEst	9.92×10 ⁻³	3.37×10 ⁻²	-1.93	-4.26	5.52×10 ⁺²	1.00×10 ⁺³	1.24×10 ⁰
D3 Hydroperoxide	1.93×10 ⁻¹	4.40×10 ⁻¹	-4.317	-6.28	6.99×10 ⁰	1.90×10 ⁻¹	9.06×10 ⁻⁴
D3 Organonitrate	1.33×10 ⁻¹	1.69×10 ⁻²	-5.536	-6.65	2.40×10 ⁻¹	1.66×10 ⁻²	1.01×10 ⁻²
D3 Ether hydroperoxide	1.70×10 ⁻¹	3.92×10 ⁻²	-3.36	-4.05	8.47×10 ⁺¹	1.95×10 ⁰	1.73×10 ⁰
D3 Ether Organonitrate	1.17×10 ⁻¹	4.27×10 ⁻³	-4.579	-6.11	2.92×10 ⁰	1.71×10 ⁻¹	1.38×10 ⁻¹
D3 Form Est 2	7.51×10 ⁻¹	1.02×10 ⁻³	-3.035	-5.56	1.24×10 ⁰	9.34×10 ⁻¹	2.05×10 ⁰
D3OH2	1.68×10 ⁻²	1.02×10 ⁻²	-2.192	-3.61	2.47×10 ⁺⁵	2.91×10 ⁺²	1.83×10 ⁺¹
D4	1.18×10 ⁰	4.90×10 ⁻¹	-6.685	-7.13	5.49×10 ⁻⁵	1.33×10 ⁻⁴	1.15×10 ⁻⁴
D4OH	1.92×10 ⁻²	2.10×10 ⁻¹	-4.56	-6.44	1.07×10 ⁰	1.09×10 ⁰	1.31×10 ⁻³
D4 Formate Ester	1.91×10 ⁻¹	1.83×10 ⁻²	-5.665	-6.67	2.40×10 ⁻³	8.60×10 ⁻³	8.88×10 ⁻³
D4OHFormEst	7.69×10 ⁻⁴	4.44×10 ⁻²	-3.499	-6.16	4.69×10 ⁺¹	3.13×10 ⁺²	1.18×10 ⁻²
D4 Hydroperoxide	2.24×10 ⁻²	3.50×10 ⁻¹	-5.886	-7.08	5.92×10 ⁻¹	4.41×10 ⁻²	1.81×10 ⁻⁴
D4 Organonitrate	1.44×10 ⁻²	5.85×10 ⁻²	-7.105	-7.23	2.04×10 ⁻²	4.14×10 ⁻³	7.65×10 ⁻⁴
D4 Ether hydroperoxide	1.97×10 ⁻²	1.40×10 ⁻¹	-4.93	-6.54	7.19×10 ⁰	4.54×10 ⁻¹	1.57×10 ⁻³

D4 Ether Organonitrate	1.42×10^{-2}	4.54×10^{-2}	-6.149	-7.02	2.48×10^{-1}	3.80×10^{-2}	1.60×10^{-3}
D4 Form Est 2	1.01×10^{-1}	6.78×10^{-3}	-4.605	-6.58	1.05×10^{-1}	1.87×10^{-1}	2.95×10^{-2}
D4OH2	1.24×10^{-3}	5.81×10^{-2}	-3.761	-6.19	$2.09 \times 10^{+4}$	$1.06 \times 10^{+2}$	8.44×10^{-3}
D5	2.18×10^{-1}	5.95×10^{-2}	-7.417	-7.61	2.37×10^{-5}	1.26×10^{-4}	3.13×10^{-4}
D5OH	2.49×10^{-3}	2.52×10^{-2}	-5.168	-6.83	4.63×10^{-1}	2.07×10^0	4.46×10^{-3}
D5 Formate Ester	3.21×10^{-2}	5.75×10^{-3}	-6.273	-7.31	1.04×10^{-3}	1.26×10^{-2}	6.47×10^{-3}
D5OHFormEst	2.39×10^{-3}	9.01×10^{-3}	-4.108	-7.25	$2.02 \times 10^{+1}$	$5.65 \times 10^{+2}$	4.74×10^{-3}
D5 Hydroperoxide	3.79×10^{-3}	1.00×10^{-1}	-6.494	-7.82	2.56×10^{-1}	6.42×10^{-2}	1.15×10^{-4}
D5 Organonitrate	5.23×10^{-3}	7.88×10^{-3}	-7.713	-7.9	8.77×10^{-3}	4.95×10^{-3}	1.21×10^{-3}
D5 Ether hydroperoxide	5.52×10^{-3}	5.42×10^{-2}	-5.538	-7.091	3.12×10^0	6.93×10^{-1}	1.14×10^{-3}
D5 Ether Organonitrate	2.30×10^{-3}	6.25×10^{-3}	-6.757	-7.62	1.07×10^{-1}	5.79×10^{-2}	2.92×10^{-3}
D5 Form Est 2	3.28×10^{-2}	1.81×10^{-3}	-5.213	-7.32	4.52×10^{-2}	2.52×10^{-1}	2.01×10^{-2}
D5OH2	1.28×10^{-4}	7.89×10^{-3}	-4.369	-6.87	$9.01 \times 10^{+3}$	$2.54 \times 10^{+2}$	1.30×10^{-2}

References

- (1) Atkinson, R.; Tuazon, E. C.; Kwok, E. S. C.; Arey, J.; Aschmann, S. M.; Bridier, I. Kinetics and Products of the Gas-Phase Reactions of $(\text{CH}_3)_4\text{Si}$, $(\text{CH}_3)_3\text{SiCH}_2\text{OH}$, $(\text{CH}_3)_3\text{SiOSi}(\text{CH}_3)_3$ and $(\text{CD}_3)_3\text{SiOSi}(\text{CD}_3)_3$ with Cl Atoms and OH Radicals. *J. Chem. Soc. Faraday Trans.* **1995**, *91* (18), 3033. <https://doi.org/10.1039/ft9959103033>.