

Supporting Information:

Development of a simple unified volatility-based scheme (SUVS) for secondary organic aerosol formation using genetic algorithms

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1. Mean molecular weights for the 10 stable species.

Table 1. Mean molecular weights for the 10 volatility-based organic species (S_{01} - S_{10})

Species	S_{01}	S_{02}	S_{03}	S_{04}	S_{05}	S_{06}	S_{07}	S_{08}	S_{09}	S_{10}
MW(g/mole)	215	214	207	198	194	168	150	97	80	57

2. List of species and genetic algorithm-derived 412 parameters in the gas phase reactions for the simple unified volatility-based scheme (SUVS)

XHC : starting organic compound of α -pinene

S_{01} - S_{10} : 10 volatility-based organic species. S_{01} is in volatility bin 1 (10^{-2} to 10^{-1} $\mu\text{g}/\text{m}^3$), S_{02} is in volatility bin 2 (10^{-1} to 10^0 $\mu\text{g}/\text{m}^3$), ... and S_{10} is in volatility bin 10 (10^6 to 10^7 $\mu\text{g}/\text{m}^3$).

$X_{01}\text{O}$ - $X_{10}\text{O}$: 10 alkoxy radicals (RO) species from 10 volatility bins

$X_{01}\text{O}_2$ - $X_{10}\text{O}_2$: 10 organic peroxy radicals (RO₂) species from 10 volatility bins

Table 2. Gas phase chemical reactions for the simple unified volatility-based scheme (SUVS)

NO.	Reactant(s) →	Product(s)	Rate constant
101	XHC + OH	→ 8.23E-04 X ₀₁ O ₂ + 5.63E-03 X ₀₂ O ₂ + 1.66E-03 X ₀₃ O ₂ + 4.40E-05 X ₀₄ O ₂ + 2.60E-02 X ₀₅ O ₂ + 3.71E-01 X ₀₆ O ₂ + 1.20E-01 X ₀₇ O ₂ + 5.80E-05 X ₀₈ O ₂ + 3.47E-01 X ₀₉ O ₂ + 1.58E-01 X ₁₀ O ₂	KOH
102	XHC + O ₃	→ 1.49E-02 X ₀₁ O ₂ + 1.90E-01 X ₀₂ O ₂ + 2.48E-02 X ₀₃ O ₂ + 1.33E-01 X ₀₄ O ₂ + 6.46E-01 X ₀₅ O ₂ + 5.74E-02 X ₀₆ O ₂ + 9.00E-06 X ₀₇ O ₂ + 1.29E-01 X ₀₈ O ₂ + 1.14E-03 X ₀₉ O ₂ + 6.16E-01 X ₁₀ O ₂	KO3
103	XHC + NO ₃	→ 2.91E-01 X ₀₁ O ₂ + 1.70E-05 X ₀₂ O ₂ + 7.00E-06 X ₀₃ O ₂ + 1.41E-01 X ₀₄ O ₂ + 3.01E-01 X ₀₅ O ₂ + 1.86E-01 X ₀₆ O ₂ + 5.32E-01 X ₀₇ O ₂ + 4.72E-01 X ₀₈ O ₂ + 1.27E-04 X ₀₉ O ₂ + 7.69E-01 X ₁₀ O ₂	KNO3
1	X ₀₁ O ₂ + NO	→ 6.90E-01 X ₀₁ O + 1.07E-01 S ₀₁ + 6.71E-01 S ₀₂	1.26E-16
2	X ₀₂ O ₂ + NO	→ 8.96E-01 X ₀₂ O + 1.10E-05 S ₀₁ + 5.82E-02 S ₀₂ + 2.77E-02 S ₀₃	2.87E-11
3	X ₀₃ O ₂ + NO	→ 4.71E-02 X ₀₃ O + 2.74E-02 S ₀₂ + 6.76E-03 S ₀₃ + 1.45E-01 S ₀₄	2.34E-12
4	X ₀₄ O ₂ + NO	→ 2.45E-02 X ₀₄ O + 2.40E-02 S ₀₃ + 2.94E-04 S ₀₄ + 9.99E-01 S ₀₅	1.16E-13
5	X ₀₅ O ₂ + NO	→ 5.30E-01 X ₀₅ O + 4.83E-01 S ₀₄ + 2.67E-01 S ₀₅ + 3.18E-01 S ₀₆	2.65E-11
6	X ₀₆ O ₂ + NO	→ 5.77E-02 X ₀₆ O + 1.50E-01 S ₀₅ + 5.37E-01 S ₀₆ + 6.64E-01 S ₀₇	2.82E-13
7	X ₀₇ O ₂ + NO	→ 1.14E-01 X ₀₇ O + 2.31E-01 S ₀₆ + 1.73E-01 S ₀₇ + 3.41E-01 S ₀₈	2.99E-16
8	X ₀₈ O ₂ + NO	→ 8.09E-01 X ₀₈ O + 6.97E-03 S ₀₇ + 8.02E-01 S ₀₈ + 2.73E-02 S ₀₉	6.91E-12
9	X ₀₉ O ₂ + NO	→ 9.99E-01 X ₀₉ O + 7.00E-06 S ₀₈ + 2.67E-04 S ₀₉ + 9.97E-01 S ₁₀	1.14E-13
10	X ₁₀ O ₂ + NO	→ 2.73E-01 X ₁₀ O + 9.88E-02 S ₀₉ + 7.25E-01 S ₁₀	4.41E-13
11	X ₀₁ O ₂ + RO ₂	→ 7.09E-02 X ₀₁ O + 9.33E-01 S ₀₁ + 1.33E-01 S ₀₂	3.29E-13
12	X ₀₂ O ₂ + RO ₂	→ 5.54E-02 X ₀₂ O + 9.37E-01 S ₀₁ + 4.93E-02 S ₀₂ + 4.11E-03 S ₀₃	3.34E-14
13	X ₀₃ O ₂ + RO ₂	→ 2.02E-01 X ₀₃ O + 9.86E-01 S ₀₂ + 4.31E-04 S ₀₃ + 5.37E-03 S ₀₄	8.50E-11
14	X ₀₄ O ₂ + RO ₂	→ 3.57E-01 X ₀₄ O + 8.09E-01 S ₀₃ + 9.92E-01 S ₀₄ + 8.17E-04 S ₀₅	3.35E-14
15	X ₀₅ O ₂ + RO ₂	→ 9.67E-01 X ₀₅ O + 2.09E-03 S ₀₄ + 2.82E-01 S ₀₅ + 9.26E-03 S ₀₆	3.34E-13
16	X ₀₆ O ₂ + RO ₂	→ 9.93E-01 X ₀₆ O + 1.97E-03 S ₀₅ + 3.41E-02 S ₀₆ + 9.96E-01 S ₀₇	1.24E-13
17	X ₀₇ O ₂ + RO ₂	→ 9.98E-01 X ₀₇ O + 7.82E-01 S ₀₆ + 2.51E-03 S ₀₇ + 1.95E-01 S ₀₈	2.94E-12
18	X ₀₈ O ₂ + RO ₂	→ 9.39E-01 X ₀₈ O + 3.29E-02 S ₀₇ + 9.99E-01 S ₀₈ + 9.45E-01 S ₀₉	5.89E-15
19	X ₀₉ O ₂ + RO ₂	→ 3.56E-01 X ₀₉ O + 4.93E-01 S ₀₈ + 7.95E-01 S ₀₉ + 1.63E-01 S ₁₀	4.43E-16
20	X ₁₀ O ₂ + RO ₂	→ 1.16E-03 X ₁₀ O + 9.16E-03 S ₀₉ + 7.67E-02 S ₁₀	5.49E-15
21	X ₀₁ O ₂ + NO ₃	→ 5.02E-01 X ₀₁ O	3.38E-15
22	X ₀₂ O ₂ + NO ₃	→ 1.85E-01 X ₀₂ O	3.29E-15
23	X ₀₃ O ₂ + NO ₃	→ 3.99E-01 X ₀₃ O	1.90E-12
24	X ₀₄ O ₂ + NO ₃	→ 1.80E-03 X ₀₄ O	1.24E-12
25	X ₀₅ O ₂ + NO ₃	→ 5.82E-03 X ₀₅ O	8.70E-11
26	X ₀₆ O ₂ + NO ₃	→ 5.47E-01 X ₀₆ O	9.95E-11
27	X ₀₇ O ₂ + NO ₃	→ 9.31E-01 X ₀₇ O	9.22E-13
28	X ₀₈ O ₂ + NO ₃	→ 3.69E-02 X ₀₈ O	4.82E-13

29	$X_{09}O_2 + NO_3 \rightarrow 2.34E-02 X_{09}O$				2.03E-16
30	$X_{10}O_2 + NO_3 \rightarrow 6.68E-04 X_{10}O$				1.90E-12
31	$X_{01}O_2 + HO_2 \rightarrow$		1.00E+00 S_{01}	+ 2.93E-01 S_{02}	1.85E-11
32	$X_{02}O_2 + HO_2 \rightarrow$	7.04E-02 S_{01}	+ 1.80E-02 S_{02}	+ 2.04E-01 S_{03}	4.99E-15
33	$X_{03}O_2 + HO_2 \rightarrow$	1.02E-03 S_{02}	+ 1.82E-02 S_{03}	+ 8.27E-02 S_{04}	4.23E-11
34	$X_{04}O_2 + HO_2 \rightarrow$	2.85E-01 S_{03}	+ 4.93E-01 S_{04}	+ 4.37E-01 S_{05}	6.87E-13
35	$X_{05}O_2 + HO_2 \rightarrow$	4.22E-03 S_{04}	+ 9.47E-01 S_{05}	+ 8.34E-03 S_{06}	1.17E-11
36	$X_{06}O_2 + HO_2 \rightarrow$	5.97E-01 S_{05}	+ 6.22E-02 S_{06}	+ 3.07E-03 S_{07}	9.74E-11
37	$X_{07}O_2 + HO_2 \rightarrow$	9.90E-01 S_{06}	+ 3.36E-02 S_{07}	+ 9.96E-01 S_{08}	1.09E-11
38	$X_{08}O_2 + HO_2 \rightarrow$	1.23E-04 S_{07}	+ 3.60E-01 S_{08}	+ 8.08E-01 S_{09}	1.85E-11
39	$X_{09}O_2 + HO_2 \rightarrow$	7.80E-05 S_{08}	+ 1.17E-04 S_{09}	+ 9.97E-01 S_{10}	9.38E-11
40	$X_{10}O_2 + HO_2 \rightarrow$	8.69E-02 S_{09}	+ 7.42E-01 S_{10}		1.20E-11
41	$X_{01}O_2 + NO_2 \rightarrow$		1.00E-06 S_{01}	+ 5.00E-05 S_{02}	2.70E-12
42	$X_{02}O_2 + NO_2 \rightarrow$	9.66E-03 S_{01}	+ 1.34E-01 S_{02}	+ 1.70E-01 S_{03}	3.02E-13
43	$X_{03}O_2 + NO_2 \rightarrow$	5.56E-01 S_{02}	+ 8.29E-01 S_{03}	+ 6.75E-01 S_{04}	2.34E-11
44	$X_{04}O_2 + NO_2 \rightarrow$	1.06E-01 S_{03}	+ 3.44E-01 S_{04}	+ 1.33E-03 S_{05}	2.32E-14
45	$X_{05}O_2 + NO_2 \rightarrow$	5.11E-01 S_{04}	+ 3.32E-04 S_{05}	+ 1.84E-01 S_{06}	7.35E-12
46	$X_{06}O_2 + NO_2 \rightarrow$	5.83E-01 S_{05}	+ 1.11E-01 S_{06}	+ 1.00E+00 S_{07}	2.94E-13
47	$X_{07}O_2 + NO_2 \rightarrow$	3.40E-01 S_{06}	+ 5.54E-04 S_{07}	+ 1.00E-05 S_{08}	1.41E-11
48	$X_{08}O_2 + NO_2 \rightarrow$	2.42E-01 S_{07}	+ 3.80E-05 S_{08}	+ 2.53E-02 S_{09}	2.04E-13
49	$X_{09}O_2 + NO_2 \rightarrow$	2.30E-04 S_{08}	+ 9.86E-03 S_{09}	+ 2.67E-01 S_{10}	9.73E-13
50	$X_{10}O_2 + NO_2 \rightarrow$	4.00E-06 S_{09}	+ 4.05E-01 S_{10}		4.73E-16
51	$X_{01}O \rightarrow$		8.85E-02 S_{01}	+ 2.21E-01 S_{02}	1.90E-16
52	$X_{02}O \rightarrow$	3.54E-01 S_{01}	+ 1.89E-01 S_{02}	+ 9.19E-01 S_{03}	2.50E-15
53	$X_{03}O \rightarrow$	5.04E-01 S_{02}	+ 9.05E-01 S_{03}	+ 4.95E-01 S_{04}	1.80E-13
54	$X_{04}O \rightarrow$	6.68E-01 S_{03}	+ 1.90E-01 S_{04}	+ 2.22E-01 S_{05}	5.08E-15
55	$X_{05}O \rightarrow$	1.60E-01 S_{04}	+ 7.47E-01 S_{05}	+ 3.97E-01 S_{06}	7.27E-16
56	$X_{06}O \rightarrow$	9.08E-01 S_{05}	+ 6.63E-01 S_{06}	+ 8.93E-01 S_{07}	1.20E-13
57	$X_{07}O \rightarrow$	3.34E-01 S_{06}	+ 1.07E-01 S_{07}	+ 2.62E-01 S_{08}	1.02E-15
58	$X_{08}O \rightarrow$	6.10E-01 S_{07}	+ 6.05E-01 S_{08}	+ 5.45E-01 S_{09}	1.18E-14
59	$X_{09}O \rightarrow$	4.04E-01 S_{08}	+ 6.40E-01 S_{09}	+ 7.23E-01 S_{10}	2.36E-15
60	$X_{10}O \rightarrow$	2.35E-01 S_{09}	+ 7.35E-01 S_{10}		1.76E-14
61	$X_{01}O \rightarrow$		1.70E-01 $X_{01}O_2$	+ 8.62E-01 $X_{02}O_2$	6.16E+06
62	$X_{02}O \rightarrow$	9.00E-06 $X_{01}O_2$	+ 2.63E-02 $X_{02}O_2$	+ 1.15E-01 $X_{03}O_2$	6.48E+06
63	$X_{03}O \rightarrow$	2.97E-02 $X_{02}O_2$	+ 7.37E-01 $X_{03}O_2$	+ 8.05E-03 $X_{04}O_2$	1.28E+06
64	$X_{04}O \rightarrow$	2.88E-02 $X_{03}O_2$	+ 1.00E-02 $X_{04}O_2$	+ 9.49E-01 $X_{05}O_2$	5.73E+05
65	$X_{05}O \rightarrow$	2.46E-04 $X_{04}O_2$	+ 1.18E-02 $X_{05}O_2$	+ 9.99E-01 $X_{06}O_2$	5.31E+06
66	$X_{06}O \rightarrow$	1.51E-03 $X_{05}O_2$	+ 9.88E-01 $X_{06}O_2$	+ 9.97E-01 $X_{07}O_2$	3.43E+06
67	$X_{07}O \rightarrow$	1.55E-03 $X_{06}O_2$	+ 9.88E-01 $X_{07}O_2$	+ 9.99E-01 $X_{08}O_2$	8.87E+05
68	$X_{08}O \rightarrow$	1.40E-01 $X_{07}O_2$	+ 6.11E-02 $X_{08}O_2$	+ 9.97E-01 $X_{09}O_2$	3.42E+06
69	$X_{09}O \rightarrow$	2.00E-04 $X_{08}O_2$	+ 9.99E-01 $X_{09}O_2$	+ 9.97E-01 $X_{10}O_2$	5.12E+05
70	$X_{10}O \rightarrow$	2.98E-02 $X_{09}O_2$	+ 6.51E-01 $X_{10}O_2$		4.59E+06

Part 3

Part 4

71	S ₀₁	→	2.48E-01 X ₀₁ O ₂ + 9.69E-01 X ₀₂ O ₂	1.15E-11 *SUN
72	S ₀₂	→	1.62E-02 X ₀₁ O ₂ + 9.64E-01 X ₀₂ O ₂ + 1.14E-01 X ₀₃ O ₂	5.44E-12 *SUN
73	S ₀₃	→	7.25E-01 X ₀₂ O ₂ + 8.92E-01 X ₀₃ O ₂ + 1.56E-01 X ₀₄ O ₂	6.17E-13 *SUN
74	S ₀₄	→	9.45E-01 X ₀₃ O ₂ + 5.78E-01 X ₀₄ O ₂ + 3.61E-01 X ₀₅ O ₂	5.40E-11 *SUN
75	S ₀₅	→	4.25E-01 X ₀₄ O ₂ + 1.77E-01 X ₀₅ O ₂ + 7.17E-01 X ₀₆ O ₂	3.50E-13 *SUN
76	S ₀₆	→	4.47E-01 X ₀₅ O ₂ + 7.59E-01 X ₀₆ O ₂ + 1.78E-01 X ₀₇ O ₂	9.43E-11 *SUN
77	S ₀₇	→	1.24E-01 X ₀₆ O ₂ + 6.20E-01 X ₀₇ O ₂ + 7.40E-01 X ₀₈ O ₂	1.51E-11 *SUN
78	S ₀₈	→	4.96E-01 X ₀₇ O ₂ + 6.69E-01 X ₀₈ O ₂ + 7.81E-01 X ₀₉ O ₂	5.79E-12 *SUN
79	S ₀₉	→	5.73E-01 X ₀₈ O ₂ + 6.23E-01 X ₀₉ O ₂ + 7.37E-01 X ₁₀ O ₂	5.34E-15 *SUN
80	S ₁₀	→	4.85E-01 X ₀₉ O ₂ + 7.07E-02 X ₁₀ O ₂	2.45E-14 *SUN
81	S ₀₁ + OH	→	1.36E-04 X ₀₁ O ₂ + 1.33E-02 X ₀₂ O ₂	9.16E-12
82	S ₀₂ + OH	→	1.04E-04 X ₀₁ O ₂ + 9.95E-04 X ₀₂ O ₂ + 6.12E-01 X ₀₃ O ₂	1.42E-11
83	S ₀₃ + OH	→	1.27E-02 X ₀₂ O ₂ + 9.98E-01 X ₀₃ O ₂ + 1.74E-02 X ₀₄ O ₂	1.95E-12
84	S ₀₄ + OH	→	3.76E-01 X ₀₃ O ₂ + 8.31E-01 X ₀₄ O ₂ + 3.85E-01 X ₀₅ O ₂	8.99E-16
85	S ₀₅ + OH	→	2.03E-02 X ₀₄ O ₂ + 3.51E-03 X ₀₅ O ₂ + 2.90E-03 X ₀₆ O ₂	2.45E-12
86	S ₀₆ + OH	→	2.86E-04 X ₀₅ O ₂ + 1.97E-03 X ₀₆ O ₂ + 9.45E-01 X ₀₇ O ₂	1.89E-11
87	S ₀₇ + OH	→	9.89E-03 X ₀₆ O ₂ + 5.95E-01 X ₀₇ O ₂ + 9.49E-01 X ₀₈ O ₂	1.31E-11
88	S ₀₈ + OH	→	9.14E-02 X ₀₇ O ₂ + 5.26E-01 X ₀₈ O ₂ + 9.98E-01 X ₀₉ O ₂	4.92E-11
89	S ₀₉ + OH	→	3.22E-01 X ₀₈ O ₂ + 9.95E-01 X ₀₉ O ₂ + 9.98E-01 X ₁₀ O ₂	3.72E-12
90	S ₁₀ + OH	→	2.41E-01 X ₀₉ O ₂ + 1.92E-01 X ₁₀ O ₂	2.11E-15
91	S ₀₁ + NO ₃	→	3.64E-01 X ₀₁ O ₂ + 3.66E-01 X ₀₂ O ₂	1.01E-16
92	S ₀₂ + NO ₃	→	8.22E-01 X ₀₁ O ₂ + 4.07E-01 X ₀₂ O ₂ + 6.94E-01 X ₀₃ O ₂	1.08E-16
93	S ₀₃ + NO ₃	→	2.93E-01 X ₀₂ O ₂ + 2.72E-01 X ₀₃ O ₂ + 2.65E-01 X ₀₄ O ₂	1.02E-16
94	S ₀₄ + NO ₃	→	2.99E-02 X ₀₃ O ₂ + 6.29E-01 X ₀₄ O ₂ + 9.85E-04 X ₀₅ O ₂	1.00E-16
95	S ₀₅ + NO ₃	→	8.32E-01 X ₀₄ O ₂ + 4.43E-01 X ₀₅ O ₂ + 2.06E-01 X ₀₆ O ₂	1.43E-16
96	S ₀₆ + NO ₃	→	1.26E-03 X ₀₅ O ₂ + 2.42E-01 X ₀₆ O ₂ + 9.97E-01 X ₀₇ O ₂	1.68E-14
97	S ₀₇ + NO ₃	→	8.92E-01 X ₀₆ O ₂ + 8.18E-01 X ₀₇ O ₂ + 9.53E-01 X ₀₈ O ₂	5.24E-16
98	S ₀₈ + NO ₃	→	2.77E-01 X ₀₇ O ₂ + 8.56E-01 X ₀₈ O ₂ + 6.27E-01 X ₀₉ O ₂	1.00E-16
99	S ₀₉ + NO ₃	→	6.41E-04 X ₀₈ O ₂ + 1.01E-01 X ₀₉ O ₂ + 3.53E-02 X ₁₀ O ₂	1.21E-14
100	S ₁₀ + NO ₃	→	2.04E-02 X ₀₉ O ₂ + 2.00E-02 X ₁₀ O ₂	8.87E-16

Part 5

Note: 1. KOH, KO₃, and KNO₃ are the reaction rate coefficients taken directly from literature or any reliable detailed chemical mechanism.

2. Photolysis reaction rate coefficient (k(71)-k(80)) are constrained by normalized sun intensity of SUN, which is 0 at night time and 1.0 at noon.