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} μg/m^3), S_{02} is in volatility bin 2 (10^{-1} to 10^{0} μg/m^3), … and S_{10} is in volatility bin 10 (10^{6} to 10^{7} μg/m^3).

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

$X_{01}O_2$ – $X_{10}O_2$: 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 $X_{03}O_2$ +	KOH
			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 $X_{10}O_2$	
102	XHC + O_3	→	1.49E-02 $X_{01}O_2$ + 1.90E-01 $X_{02}O_2$ + 2.48E-02 $X_{03}O_2$ +	KO3
			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 $X_{10}O_2$	
103	XHC + NO_3	→	2.91E-01 $X_{01}O_2$ + 1.70E-05 $X_{02}O_2$ + 7.00E-06 $X_{03}O_2$ +	KNO3
			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 $X_{10}O_2$	
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

Part 1

Part 2

29	$X_{09}O_2 + NO_3$	→	2.34E-02	$X_{09}O$						2.03E-16	
30	$X_{10}O_2 + NO_3$	→	6.68E-04	$X_{10}O$						1.90E-12	
31	$X_{01}O_2 + HO_2$	→			1.00E+00	S_{01}	+	2.93E-01	S_{02}	1.85E-11	
32	$X_{02}O_2 + HO_2$	→	7.04E-02	S_{01}	+ 1.80E-02	S_{02}	+	2.04E-01	S_{03}	4.99E-15	**Part 3**
33	$X_{03}O_2 + HO_2$	→	1.02E-03	S_{02}	+ 1.82E-02	S_{03}	+	8.27E-02	S_{04}	4.23E-11	
34	$X_{04}O_2 + HO_2$	→	2.85E-01	S_{03}	+ 4.93E-01	S_{04}	+	4.37E-01	S_{05}	6.87E-13	
35	$X_{05}O_2 + HO_2$	→	4.22E-03	S_{04}	+ 9.47E-01	S_{05}	+	8.34E-03	S_{06}	1.17E-11	
36	$X_{06}O_2 + HO_2$	→	5.97E-01	S_{05}	+ 6.22E-02	S_{06}	+	3.07E-03	S_{07}	9.74E-11	
37	$X_{07}O_2 + HO_2$	→	9.90E-01	S_{06}	+ 3.36E-02	S_{07}	+	9.96E-01	S_{08}	1.09E-11	
38	$X_{08}O_2 + HO_2$	→	1.23E-04	S_{07}	+ 3.60E-01	S_{08}	+	8.08E-01	S_{09}	1.85E-11	
39	$X_{09}O_2 + HO_2$	→	7.80E-05	S_{08}	+ 1.17E-04	S_{09}	+	9.97E-01	S_{10}	9.38E-11	
40	$X_{10}O_2 + HO_2$	→	8.69E-02	S_{09}	+ 7.42E-01	S_{10}				1.20E-11	
41	$X_{01}O_2 + NO_2$	→			1.00E-06	S_{01}	+	5.00E-05	S_{02}	2.70E-12	
42	$X_{02}O_2 + NO_2$	→	9.66E-03	S_{01}	+ 1.34E-01	S_{02}	+	1.70E-01	S_{03}	3.02E-13	
43	$X_{03}O_2 + NO_2$	→	5.56E-01	S_{02}	+ 8.29E-01	S_{03}	+	6.75E-01	S_{04}	2.34E-11	
44	$X_{04}O_2 + NO_2$	→	1.06E-01	S_{03}	+ 3.44E-01	S_{04}	+	1.33E-03	S_{05}	2.32E-14	
45	$X_{05}O_2 + NO_2$	→	5.11E-01	S_{04}	+ 3.32E-04	S_{05}	+	1.84E-01	S_{06}	7.35E-12	
46	$X_{06}O_2 + NO_2$	→	5.83E-01	S_{05}	+ 1.11E-01	S_{06}	+	1.00E+00	S_{07}	2.94E-13	
47	$X_{07}O_2 + NO_2$	→	3.40E-01	S_{06}	+ 5.54E-04	S_{07}	+	1.00E-05	S_{08}	1.41E-11	
48	$X_{08}O_2 + NO_2$	→	2.42E-01	S_{07}	+ 3.80E-05	S_{08}	+	2.53E-02	S_{09}	2.04E-13	
49	$X_{09}O_2 + NO_2$	→	2.30E-04	S_{08}	+ 9.86E-03	S_{09}	+	2.67E-01	S_{10}	9.73E-13	
50	$X_{10}O_2 + NO_2$	→	4.00E-06	S_{09}	+ 4.05E-01	S_{10}				4.73E-16	
51	$X_{01}O$	→			8.85E-02	S_{01}	+	2.21E-01	S_{02}	1.90E-16	
52	$X_{02}O$	→	3.54E-01	S_{01}	+ 1.89E-01	S_{02}	+	9.19E-01	S_{03}	2.50E-15	
53	$X_{03}O$	→	5.04E-01	S_{02}	+ 9.05E-01	S_{03}	+	4.95E-01	S_{04}	1.80E-13	
54	$X_{04}O$	→	6.68E-01	S_{03}	+ 1.90E-01	S_{04}	+	2.22E-01	S_{05}	5.08E-15	
55	$X_{05}O$	→	1.60E-01	S_{04}	+ 7.47E-01	S_{05}	+	3.97E-01	S_{06}	7.27E-16	
56	$X_{06}O$	→	9.08E-01	S_{05}	+ 6.63E-01	S_{06}	+	8.93E-01	S_{07}	1.20E-13	
57	$X_{07}O$	→	3.34E-01	S_{06}	+ 1.07E-01	S_{07}	+	2.62E-01	S_{08}	1.02E-15	
58	$X_{08}O$	→	6.10E-01	S_{07}	+ 6.05E-01	S_{08}	+	5.45E-01	S_{09}	1.18E-14	
59	$X_{09}O$	→	4.04E-01	S_{08}	+ 6.40E-01	S_{09}	+	7.23E-01	S_{10}	2.36E-15	
60	$X_{10}O$	→	2.35E-01	S_{09}	+ 7.35E-01	S_{10}				1.76E-14	**Part 4**
61	$X_{01}O$	→			1.70E-01	$X_{01}O_2$	+	8.62E-01	$X_{02}O_2$	6.16E+06	
62	$X_{02}O$	→	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	$X_{03}O$	→	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	$X_{04}O$	→	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	$X_{05}O$	→	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	$X_{06}O$	→	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	$X_{07}O$	→	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	$X_{08}O$	→	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	$X_{09}O$	→	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	$X_{10}O$	→	2.98E-02	$X_{09}O_2$	+ 6.51E-01	$X_{10}O_2$				4.59E+06	

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.