Article

Fixed- and Variable-Temperature Kinetic Models to Predict Evaporation of Petroleum Distillates for Fire Debris Applications

John W. McIlroy [1,†], Ruth Waddell Smith [2,*] and Victoria L. McGuffin [1,*]

[1] Department of Chemistry, Michigan State University, East Lansing, MI 48824, USA
[2] Forensic Science Program, School of Criminal Justice, Michigan State University, East Lansing, MI 48824, USA
[†] Current address: Drug Enforcement Administration, 10150 Technology Blvd., Dallas, TX 75220, USA
* Correspondence: rwsmith@msu.edu (R.W.S.); mcguffin@msu.edu (V.L.M.); Tel.: +1-517-353-5283 (R.W.S.); +1-517-353-1091 (V.L.M.)

Table S1a. Selected compounds monitored during evaporation of diesel fuel for development of fixed-temperature and variable-temperature models. The following information is listed for each compound: Peak number in Tables S2a–S6b (Peak #), compound identity, compound class, the mass-to-charge (m/z) ratio of the extracted ion chromatogram (EIC) used to quantify the compound, the retention time (t^{T_R}), the boiling point (T_b), and retention index (I^T) before and after correction.

Peak #	Compound	Class	m/z	t^{T_R} (min)	T_b (K) [1]	I^T	I^T Corrected [2]
1	2-Methyl heptane	Branched Alkane	57	3.398			
2	Octane	Normal Alkane	57	3.748	399	800	800
3	4-Methyl octane	Branched Alkane	57	4.814	415	862	862
4	3-Methyl octane	Branched Alkane	57	4.948	417	869	869
5	Nonane	Normal Alkane	57	5.479	424	900	900
6	Dimethyl octane isomer	Branched Alkane	57	6.248		933	933
7	Ethyl methyl heptane isomer	Branched Alkane	57	6.411		940	940
8	Methyl nonane isomer	Branched Alkane	57	6.883		960	960
9	Unidentified	Branched Alkane	57	7.105		970	970
10	Decane	Normal Alkane	57	7.816	447	1000	1000
11	4-Methyl decane	Branched Alkane	57	8.434	460	1024	1024
12	5-Methyl decane	Branched Alkane	57	9.326		1058	1058
13	2-Methyl decane	Branched Alkane	57	9.506	462	1064	1064
14	3-Methyl decane	Branched Alkane	57	9.670		1071	1071
15	Undecane	Normal Alkane	57	10.439	468	1100	1100
16	Unidentified	Branched Alkane	57	11.960		1155	1155
17	Methyl undecane isomer	Branched Alkane	57	12.217		1165	1165
18	Unidentified	Branched Alkane	57	12.392		1171	1171
19	Dodecane	Normal Alkane	57	13.184	489	1200	1200
20	2,6-Dimethyl undecane	Branched Alkane	57	13.616		1216	1216
21	Unidentified	Branched Alkane	57	14.618		1254	1254
22	Unidentified	Branched Alkane	57	15.213		1276	1276
23	Tridecane	Normal Alkane	57	15.848	507	1300	1300
24	Unidentified	Branched Alkane	57	17.527		1365	1365
25	2,6,10-Trimethyl decane	Branched Alkane	57	17.900		1379	1379
26	Tetradecane	Normal Alkane	57	18.430	523	1400	1400
27	Unidentified	Branched Alkane	57	20.027		1465	1465
28	Pentadecane	Normal Alkane	57	20.890	540	1500	1500
29	Hexadecane	Normal Alkane	57	23.186	554	1600	1600
30	2,6,10-Trimethyl pentadecane	Branched Alkane	57	24.369		1654	1654
31	Heptadecane	Normal Alkane	57	25.395	575	1700	1700
32	Pristane	Branched Alkane	57	25.628		1711	1711
33	Octadecane	Normal Alkane	57	27.488	589	1800	1800

Peak #	Compound	Class	*m/z*	t^{T_R} (min)	T_b (K) [1]	I^T	I^T Corrected [2]
34	Phytane	Branched Alkane	57	27.791		1815	1815
35	Nonadecane	Normal Alkane	57	29.539		1900	1900
36	Eicosane	Normal Alkane	57	31.400	616	2000	2000
37	Heneicosane	Normal Alkane	57	33.276	635	2100	2100
38	Methyl cyclohexane	Branched Alkane	83	2.856	374		
39	Ethyl cyclohexane	Branched Alkane	83	4.226	405	828	828
40	Propyl cyclohexane	Branched Alkane	83	6.067	429	925	925
41	Butyl cyclohexane	Branched Alkane	83	8.527	453	1027	1027
42	Pentyl cyclohexane	Branched Alkane	83	11.272	477	1130	1130
43	Hexyl cyclohexane	Branched Alkane	83	14.288	498	1241	1241
44	Heptyl cyclohexane	Branched Alkane	83	16.833	510	1338	1338
45	Octyl cyclohexane	Branched Alkane	83	19.462	528	1442	1442
46	Toluene	Alkyl Aromatic	91	3.194	384		
47	Ethyl benzene	Alkyl Aromatic	91	4.511	409	844	827
48	*m*/*p*-Xylene	Alkyl Aromatic	91	4.663	412	853	836
49	*o*-Xylene	Alkyl Aromatic	91	5.071	417	876	859
50	Propyl benzene	Alkyl Aromatic	91	6.365	432	938	921
51	Butyl benzene	Alkyl Aromatic	91	8.871	456	1040	1023
52	Unidentified	Alkyl Aromatic	91	10.171		1090	1073
53	1,2,3,4-Tetrahydro-naphthalene	Polycyclic Hydrocarbon	91	11.465	490	1137	1120
54	Pentyl benzene	Alkyl Aromatic	91	11.576		1141	1124
55	Methyl tetralin isomer	Polycyclic Hydrocarbon	91	12.980		1193	1176
56	Unidentified	Polycyclic Hydrocarbon	91	17.066		1347	1330
57	Unidentified	Polycyclic Hydrocarbon	91	19.660		1450	1433
58	Ethyl methyl benzene isomer	Alkyl Aromatic	105	6.534		945	928
59	1,3,5-Trimethyl benzene	Alkyl Aromatic	105	6.720	438	953	936
60	Ethyl methyl benzene isomer	Alkyl Aromatic	105	6.930		962	945
61	1,2,4-Trimethyl benzene	Alkyl Aromatic	105	7.291	442	978	961
62	Unidentified	Alkyl Aromatic	105	7.734		996	979
63	1,2,3-Trimethyl benzene	Alkyl Aromatic	105	7.950	449	1005	988

Peak #	Compound	Class	*m/z*	t^{T}_{R} (min)	T_b (K) [1]	I^T	I^T Corrected [2]
64	Methyl propyl benzene isomer	Alkyl Aromatic	105	8.754		1036	1019
65	Methyl propyl benzene isomer	Alkyl Aromatic	105	8.854		1040	1023
66	Methyl propyl benzene isomer	Alkyl Aromatic	105	9.139		1050	1033
67	Unidentified	Alkyl Aromatic	105	10.113		1088	1071
68	Indane	Polycyclic Hydrocarbon	117	8.212	450	1015	998
69	Methyl indane isomer	Polycyclic Hydrocarbon	117	9.565		1067	1050
70	Unidentified	Polycyclic Hydrocarbon	117	10.958		1119	1102
71	Unidentified	Polycyclic Hydrocarbon	117	11.220		1128	1111
72	Unidentified	Polycyclic Hydrocarbon	117	13.516		1212	1195
73	Methyl tetralin isomer	Polycyclic Hydrocarbon	117	14.303	507	1242	1225
74	Methyl tetralin isomer	Polycyclic Hydrocarbon	117	14.974		1267	1250
75	Methyl tetralin isomer	Polycyclic Hydrocarbon	117	15.760		1297	1280
76	Methyl tetralin isomer	Polycyclic Hydrocarbon	117	16.349		1319	1302
77	Methyl tetralin isomer	Polycyclic Hydrocarbon	117	17.591		1368	1351
78	Naphthalene	Polycyclic Hydrocarbon	128	11.949	490	1155	1138

[1] Source: Brown, R. L.; Stein, S. E., Boiling Point Data. In *NIST Chemistry WebBook, NIST Standard Reference Database Number 69*, Linstrom, P. J.; Mallard, W. G., Eds. National Institute of Standards and Technology, Mass Spec Data Center: Gaithersburg, MD, 2011. http//webbook.nist.gov, (retrieved February 26, 2014); Vol. February 26, 2014. [2] For compounds in the alkyl aromatic and polycyclic aromatic classes, retention index is corrected using the McReynolds constant for benzene on 100% poly(dimethylsiloxane) stationary phase. I^T corrected = I^T–17.

Table S1b. Selected compounds monitored during evaporation of diesel fuel for validation of fixed-temperature and variable-temperature models. The following information is listed for each compound: Peak number in Tables S2a–S6b (Peak #), compound identity, compound class, the mass-to-charge (*m*/*z*) ratio of the extracted ion chromatogram (EIC) used to quantify the compound, the retention time (t^{T}_{R}), the boiling point (T_b), and retention index (I^T) before and after correction.

Peak #	Class	*m*/*z*	t^{T}_{R} (min)	I^T	I^T Corrected [1]
79	Branched Alkane	57	12.094	1160	1160
80	Branched Alkane	57	15.078	1271	1271
81	Alkyl Aromatic	105	5.723	910	893
82	Alkyl Aromatic	105	11.605	1142	1125
83	Alkyl Aromatic	105	11.832	1151	1134
84	Alkyl Aromatic	117	14.641	1255	1238
85	Polycyclic Hydrocarbon	117	16.728	1334	1317
86	Branched Alkane	97	3.800	803	803
87	Branched Alkane	97	5.205	884	884
88	Branched Alkane	97	5.578	904	904
89	Branched Alkane	97	7.326	979	979
90	Branched Alkane	97	7.390	982	982
91	Branched Alkane	97	7.647	993	993
92	Branched Alkane	97	9.943	1081	1081
93	Branched Alkane	97	10.241	1092	1092
94	Alkyl Aromatic	119	8.002	1007	990
95	Alkyl Aromatic	119	8.084	1010	993
96	Alkyl Aromatic	119	8.864	1033	1016
97	Alkyl Aromatic	119	8.941	1043	1026
98	Alkyl Aromatic	119	9.617	1069	1052
99	Alkyl Aromatic	119	10.650	1104	1087
100	Alkyl Aromatic	119	11.360	1134	1117
101	Alkyl Aromatic	119	11.686	1145	1128
102	Alkyl Aromatic	119	11.797	1149	1132
103	Alkyl Aromatic	119	12.036	1158	1141
104	Polycyclic Hydrocarbon	137	10.532	1103	1086
105	Polycyclic Hydrocarbon	137	13.645	1217	1200
106	Polycyclic Hydrocarbon	137	13.907	1227	1210

[1] For compounds in the alkyl aromatic and polycyclic aromatic classes, retention index is corrected using the McReynolds constant for benzene on 100% poly(dimethylsiloxane) stationary phase. I^T corrected = I^T −17.

Table S2a. For model development, the experimental rate constant (k_{exp}), characteristic lifetime (τ), and the number of τ in 300 h for selected compounds monitored during the evaporation of diesel fuel at 5 °C. The predicted rate constant (k_{pred}) and absolute percent error (APE) were calculated using the fixed-temperature (Fixed T) and variable-temperature (Variable T) models. Compounds with τ < 0.5 in 300 h were excluded from the models (peaks 16–37, 43–45, 72–77). Several compounds had retention indices less than 800 (peaks 1, 38, 46) and were also excluded, as the retention index could not be accurately determined.

Peak #	k_{exp} (h^{-1})	τ (h)	# τ in 300 h	k_{pred} Fixed T	k_{pred} Variable T	APE Fixed T	APE Variable T
1	1.83E-01	5.5	54.9				
2	1.28E-01	7.8	38.3	1.10E-01	7.36E-02	14.1	42.4
3	5.04E-02	19.8	15.1	5.49E-02	3.90E-02	9.0	22.6
4	4.97E-02	20.1	14.9	5.04E-02	3.60E-02	1.3	27.5
5	3.34E-02	29.9	10.0	3.57E-02	2.63E-02	6.7	21.4
6	2.32E-02	43.1	7.0	2.46E-02	1.87E-02	6.2	19.3
7	2.27E-02	44.0	6.8	2.28E-02	1.74E-02	0.4	23.2
8	1.63E-02	61.3	4.9	1.82E-02	1.42E-02	11.4	13.2
9	1.48E-02	67.7	4.4	1.63E-02	1.28E-02	10.5	13.1
10	1.02E-02	98.5	3.0	1.16E-02	9.38E-03	14.1	7.6
11	8.24E-03	121.3	2.5	8.90E-03	7.36E-03	7.9	10.7
12	5.56E-03	179.9	1.7	6.07E-03	5.19E-03	9.2	6.7
13	4.98E-03	201.0	1.5	5.62E-03	4.83E-03	12.9	2.8
14	4.79E-03	208.6	1.4	5.24E-03	4.53E-03	9.2	5.4
15	3.13E-03	320.0	0.9	3.77E-03	3.35E-03	20.5	7.3
38	4.40E-01	2.3	132.1				
39	1.04E-01	9.6	31.3	8.05E-02	5.54E-02	23.0	47.0
40	2.98E-02	33.5	8.9	2.69E-02	2.03E-02	9.9	32.0
41	9.46E-03	105.7	2.8	8.55E-03	7.10E-03	9.6	24.9
42	2.86E-03	350.1	0.9	2.68E-03	2.45E-03	6.2	14.1
46	3.04E-01	3.3	91.3				
47	9.70E-02	10.3	29.1	8.10E-02	5.57E-02	16.5	42.6
48	7.42E-02	13.5	22.3	7.34E-02	5.09E-02	1.1	31.4
49	5.84E-02	17.1	17.5	5.63E-02	3.99E-02	3.6	31.7
50	2.94E-02	34.0	8.8	2.82E-02	2.12E-02	4.0	27.9
51	8.80E-03	113.6	2.6	8.93E-03	7.39E-03	1.4	16.1
52	5.00E-03	200.1	1.5	5.12E-03	4.44E-03	2.4	11.2
53	3.36E-03	297.5	1.0	3.00E-03	2.72E-03	10.9	19.1
54	2.74E-03	365.0	0.8	2.86E-03	2.61E-03	4.5	4.9
55	1.70E-03	589.0	0.5	1.61E-03	1.54E-03	5.1	9.3
58	2.42E-02	41.3	7.3	2.60E-02	1.97E-02	7.3	18.8
59	1.78E-02	56.3	5.3	2.38E-02	1.81E-02	33.8	2.0
60	2.02E-02	49.6	6.0	2.15E-02	1.65E-02	6.6	18.1
61	1.64E-02	61.0	4.9	1.81E-02	1.41E-02	10.1	14.1
62	1.52E-02	66.0	4.5	1.46E-02	1.16E-02	3.7	23.5
63	1.19E-02	84.1	3.6	1.33E-02	1.06E-02	11.4	10.8
64	8.57E-03	116.7	2.6	9.39E-03	7.74E-03	9.5	9.7
65	8.80E-03	113.6	2.6	8.99E-03	7.44E-03	2.2	15.5

Peak #	k_{exp} (h^{-1})	τ (h)	# τ in 300 h	k_{pred} Fixed T	k_{pred} Variable T	APE Fixed T	APE Variable T
66	7.67E-03	130.3	2.3	7.96E-03	6.65E-03	3.7	13.3
67	5.00E-03	200.1	1.5	5.24E-03	4.54E-03	4.9	9.2
68	1.40E-02	71.3	4.2	1.18E-02	9.57E-03	15.5	31.7
69	7.43E-03	134.6	2.2	6.63E-03	5.63E-03	10.7	24.2
70	4.08E-03	245.1	1.2	3.69E-03	3.29E-03	9.6	19.5
71	3.77E-03	265.6	1.1	3.31E-03	2.98E-03	12.0	20.9
78	3.56E-03	281.2	1.1	2.46E-03	2.27E-03	30.9	36.3

Table S2b. For model validation, the experimental rate constant (k_{exp}), characteristic lifetime (τ), and the number of τ in 300 h for selected compounds in diesel fuel evaporated at 5 °C. The predicted rate constant (k_{pred}) and absolute percent error (APE) were calculated using the fixed-temperature (Fixed T) and variable-temperature (Variable T) models. Compounds with τ < 0.5 in 300 h were excluded from the models (peaks 80, 84, 85, 105, 106).

Peak #	k_{exp} (h^{-1})	τ (h)	# τ in 300 h	k_{pred} Fixed T	k_{pred} Variable T	APE Fixed T	APE Variable T
79	1.52E-03	657.5	0.5	1.91E-03	1.80E-03	25.8	18.5
81	2.94E-02	34.1	8.8	3.84E-02	2.81E-02	30.7	4.3
82	1.86E-03	538.5	0.6	2.83E-03	2.58E-03	52.4	38.9
83	1.90E-03	526.6	0.6	2.58E-03	2.37E-03	35.7	24.7
86	1.51E-01	6.6	45.3	1.06E-01	7.13E-02	29.8	52.8
87	4.52E-02	22.1	13.6	4.26E-02	3.09E-02	5.7	31.6
88	3.88E-02	25.8	11.6	3.40E-02	2.52E-02	12.3	35.1
89	1.45E-02	69.1	4.3	1.47E-02	1.16E-02	1.5	19.5
90	1.50E-02	66.7	4.5	1.42E-02	1.13E-02	5.1	24.5
91	1.39E-02	71.8	4.2	1.26E-02	1.01E-02	9.7	27.4
92	4.75E-03	210.7	1.4	4.66E-03	4.07E-03	1.9	14.2
93	4.66E-03	214.4	1.4	4.10E-03	3.62E-03	12.1	22.3
94	1.19E-02	83.8	3.6	1.30E-02	1.04E-02	8.6	12.9
95	1.14E-02	87.4	3.4	1.25E-02	1.01E-02	9.3	12.0
96	9.01E-03	111.0	2.7	9.67E-03	7.95E-03	7.3	11.8
97	7.14E-03	140.0	2.1	8.67E-03	7.19E-03	21.3	0.7
98	6.07E-03	164.7	1.8	6.49E-03	5.51E-03	6.8	9.2
99	3.85E-03	260.1	1.2	4.36E-03	3.83E-03	13.3	0.4
100	3.08E-03	324.8	0.9	3.13E-03	2.83E-03	1.6	8.2
101	2.51E-03	398.6	0.8	2.74E-03	2.50E-03	9.1	0.3
102	2.32E-03	431.3	0.7	2.62E-03	2.40E-03	12.8	3.5
103	2.08E-03	480.5	0.6	2.37E-03	2.19E-03	13.9	5.4
104	4.13E-03	242.0	1.2	4.39E-03	3.86E-03	6.3	6.7
107	8.41E-03	119.0	2.5	8.26E-03	6.88E-03	0.7	18.1

Table S3a. For model development, the experimental rate constant (k_{exp}), characteristic lifetime (τ), and the number of τ in 300 h for selected compounds monitored during the evaporation of diesel fuel at 10 °C. The predicted rate constant (k_{pred}) and absolute percent error (APE) were calculated using the fixed-temperature (Fixed T) and variable-temperature (Variable T) models. Compounds with τ < 0.5 in 300 h were excluded from the models (peaks 19–37, 43–45, 73–77). Several compounds had retention indices lower than 800 (peaks 1, 38, 46) and were also excluded, as the retention index could not be accurately determined.

Peak #	k_{exp} (h^{-1})	τ (h)	# τ in 300 h	k_{pred} Fixed T	k_{pred} Variable T	APE Fixed T	APE Variable T
1	2.13E-01	4.7	63.8				
2	1.51E-01	6.6	45.2	1.05E-01	1.10E-01	30.2	26.8
3	5.49E-02	18.2	16.5	5.50E-02	5.85E-02	0.2	6.6
4	5.33E-02	18.8	16.0	5.07E-02	5.40E-02	4.9	1.4
5	3.47E-02	28.8	10.4	3.67E-02	3.94E-02	5.7	13.4
6	2.45E-02	40.8	7.4	2.60E-02	2.81E-02	5.9	14.4
7	2.35E-02	42.5	7.1	2.41E-02	2.61E-02	2.7	11.2
8	1.72E-02	58.1	5.2	1.95E-02	2.12E-02	13.4	23.4
9	1.59E-02	62.8	4.8	1.77E-02	1.93E-02	10.9	20.9
10	1.08E-02	92.5	3.2	1.28E-02	1.41E-02	18.6	30.2
11	9.51E-03	105.2	2.9	1.00E-02	1.10E-02	5.2	16.2
12	6.82E-03	146.6	2.0	6.99E-03	7.78E-03	2.5	14.1
13	6.17E-03	162.1	1.9	6.50E-03	7.25E-03	5.5	17.6
14	6.06E-03	164.9	1.8	6.09E-03	6.80E-03	0.4	12.1
15	4.25E-03	235.5	1.3	4.47E-03	5.03E-03	5.3	18.4
16	2.31E-03	433.8	0.7	2.50E-03	2.84E-03	8.3	23.2
17	1.99E-03	502.3	0.6	2.26E-03	2.58E-03	13.6	29.6
18	1.90E-03	526.1	0.6	2.11E-03	2.42E-03	11.3	27.1
38	5.10E-01	2.0	153.1				
39	1.13E-01	8.9	33.8	7.87E-02	8.30E-02	30.1	26.2
40	3.07E-02	32.6	9.2	2.82E-02	3.04E-02	8.3	1.0
41	1.00E-02	100.0	3.0	9.63E-03	1.06E-02	3.7	6.4
42	3.80E-03	263.1	1.1	3.25E-03	3.68E-03	14.5	3.3
46	3.62E-01	2.8	108.7				
47	9.57E-02	10.5	28.7	7.91E-02	8.35E-02	17.3	12.7
48	7.23E-02	13.8	21.7	7.21E-02	7.63E-02	0.3	5.4
49	5.75E-02	17.4	17.3	5.63E-02	5.98E-02	2.1	4.0
50	2.83E-02	35.3	8.5	2.95E-02	3.18E-02	4.1	12.3
51	9.41E-03	106.2	2.8	1.00E-02	1.11E-02	6.6	17.7
52	5.55E-03	180.2	1.7	5.96E-03	6.65E-03	7.4	19.9
53	4.17E-03	239.7	1.3	3.61E-03	4.08E-03	13.5	2.3
54	3.59E-03	278.7	1.1	3.46E-03	3.91E-03	3.6	8.9
55	2.30E-03	434.1	0.7	2.02E-03	2.31E-03	12.4	0.2
58	2.33E-02	42.9	7.0	2.73E-02	2.95E-02	17.1	26.4
59	1.79E-02	56.0	5.4	2.51E-02	2.72E-02	40.6	52.1
60	1.99E-02	50.1	6.0	2.28E-02	2.48E-02	14.5	24.2
61	1.58E-02	63.1	4.8	1.94E-02	2.11E-02	22.5	33.3
62	1.47E-02	67.9	4.4	1.59E-02	1.74E-02	8.1	18.1

Peak #	k_{exp} (h^{-1})	τ (h)	# τ in 300 h	k_{pred} Fixed T	k_{pred} Variable T	APE Fixed T	APE Variable T
63	1.26E-02	79.5	3.8	1.45E-02	1.59E-02	15.4	26.4
64	9.24E-03	108.2	2.8	1.05E-02	1.16E-02	13.8	25.6
65	9.11E-03	109.8	2.7	1.01E-02	1.12E-02	10.9	22.5
66	8.75E-03	114.3	2.6	9.01E-03	9.97E-03	3.0	14.0
67	6.09E-03	164.3	1.8	6.10E-03	6.81E-03	0.1	11.8
68	1.36E-02	73.6	4.1	1.31E-02	1.44E-02	3.7	5.7
69	8.00E-03	125.1	2.4	7.60E-03	8.44E-03	5.0	5.5
70	5.05E-03	198.1	1.5	4.38E-03	4.93E-03	13.1	2.3
71	4.74E-03	211.0	1.4	3.96E-03	4.47E-03	16.3	5.7
72	1.77E-03	564.6	0.5	1.64E-03	1.88E-03	7.6	6.2
78	4.82E-03	207.7	1.4	3.00E-03	3.40E-03	37.7	29.4

Table S3b. For model validation, the experimental rate constant (k_{exp}), characteristic lifetime (τ), and the number of τ in 300 h for selected compounds in diesel fuel evaporated at 10 °C. The predicted rate constant (k_{pred}) and absolute percent error (APE) were calculated using the fixed-temperature (Fixed T) and variable-temperature (Variable T) models. Compounds with τ < 0.5 in 300 h were excluded from the models (peaks 80, 84, 85, 105, 106).

Peak #	k_{exp} (h^{-1})	τ (h)	# τ in 300 h	k_{pred} Fixed T	k_{pred} Variable T	APE Fixed T	APE Variable T
79	2.18E-03	459.2	0.7	2.37E-03	2.70E-03	8.9	24.1
81	3.84E-02	26.0	11.5	3.93E-02	4.21E-02	2.4	9.7
82	3.51E-03	284.7	1.1	3.42E-03	3.87E-03	2.6	10.1
83	3.39E-03	295.2	1.0	3.14E-03	3.55E-03	7.4	4.8
86	1.61E-01	6.2	48.2	1.02E-01	1.07E-01	36.6	33.5
87	4.63E-02	21.6	13.9	4.34E-02	4.64E-02	6.2	0.2
88	3.91E-02	25.6	11.7	3.51E-02	3.77E-02	10.2	3.5
89	1.45E-02	68.8	4.4	1.60E-02	1.75E-02	10.0	20.2
90	1.50E-02	66.8	4.5	1.55E-02	1.70E-02	3.6	13.3
91	1.39E-02	72.0	4.2	1.38E-02	1.52E-02	0.4	9.1
92	5.87E-03	170.4	1.8	5.46E-03	6.10E-03	7.0	4.0
93	5.65E-03	176.9	1.7	4.84E-03	5.43E-03	14.3	3.9
94	1.19E-02	84.2	3.6	1.42E-02	1.56E-02	19.7	31.2
95	1.15E-02	86.8	3.5	1.38E-02	1.51E-02	19.4	30.9
96	9.48E-03	105.4	2.8	1.08E-02	1.19E-02	14.0	25.7
97	7.92E-03	126.2	2.4	9.76E-03	1.08E-02	23.2	36.1
98	6.98E-03	143.2	2.1	7.44E-03	8.27E-03	6.6	18.4
99	4.83E-03	207.0	1.4	5.13E-03	5.74E-03	6.1	18.9
100	3.96E-03	252.3	1.2	3.76E-03	4.24E-03	5.2	6.9
101	3.43E-03	291.5	1.0	3.32E-03	3.75E-03	3.3	9.4
102	3.14E-03	318.3	0.9	3.18E-03	3.60E-03	1.1	14.5
103	2.87E-03	348.8	0.9	2.90E-03	3.29E-03	1.1	14.8
104	4.81E-03	207.7	1.4	5.16E-03	5.78E-03	7.2	20.1
107	8.78E-03	113.9	2.6	9.33E-03	1.03E-02	6.3	17.6

Table S4a. For model development, the experimental rate constant (k_{exp}), characteristic lifetime (τ), and the number of τ in 300 h for selected compounds monitored during the evaporation of diesel fuel at 20 °C. The predicted rate constant (k_{pred}) and absolute percent error (APE) were calculated using the fixed-temperature (Fixed T) and variable-temperature (Variable T) models. Compounds with τ < 0.5 in 300 h were excluded from the models (peaks 23–37, 44, 45, 57). Several compounds had retention indices lower than 800 (peaks 1, 38, 46) and were also excluded, as the retention index could not be accurately determined.

Peak #	k_{exp} (h^{-1})	τ (h)	# τ in 300 h	k_{pred} Fixed T	k_{pred} Variable T	APE Fixed T	APE Variable T
1	3.08E-01	3.2	92.5				
2	2.26E-01	4.4	67.7	1.92E-01	2.31E-01	14.9	2.3
3	1.08E-01	9.3	32.4	1.01E-01	1.22E-01	6.5	13.6
4	9.72E-02	10.3	29.2	9.31E-02	1.13E-01	4.2	16.4
5	6.58E-02	15.2	19.8	6.75E-02	8.25E-02	2.6	25.3
6	4.53E-02	22.1	13.6	4.79E-02	5.88E-02	5.7	29.8
7	4.39E-02	22.8	13.2	4.45E-02	5.47E-02	1.3	24.5
8	3.30E-02	30.3	9.9	3.60E-02	4.44E-02	9.2	34.6
9	2.88E-02	34.7	8.7	3.26E-02	4.03E-02	13.2	39.7
10	2.01E-02	49.8	6.0	2.38E-02	2.95E-02	18.2	46.6
11	1.64E-02	61.1	4.9	1.86E-02	2.31E-02	13.4	41.2
12	1.18E-02	84.5	3.5	1.30E-02	1.63E-02	10.0	37.7
13	1.05E-02	95.2	3.2	1.21E-02	1.52E-02	15.3	44.4
14	1.02E-02	97.6	3.1	1.13E-02	1.42E-02	10.8	38.9
15	7.46E-03	134.1	2.2	8.35E-03	1.05E-02	12.0	41.1
16	4.56E-03	219.1	1.4	4.68E-03	5.95E-03	2.5	30.3
17	3.91E-03	255.5	1.2	4.24E-03	5.40E-03	8.5	38.0
18	3.87E-03	258.4	1.2	3.97E-03	5.06E-03	2.6	30.7
19	2.20E-03	453.8	0.7	2.94E-03	3.76E-03	33.3	70.5
20	2.02E-03	495.6	0.6	2.48E-03	3.18E-03	22.9	57.6
21	1.30E-03	771.9	0.4	1.67E-03	2.16E-03		
22	8.46E-04	1182.5	0.3	1.33E-03	1.72E-03		
23	4.90E-04	2041.5	0.1	1.03E-03	1.34E-03		
38	6.21E-01	1.6	186.4				
39	1.81E-01	5.5	54.3	1.44E-01	1.74E-01	20.4	3.9
40	5.86E-02	17.1	17.6	5.19E-02	6.37E-02	11.4	8.6
41	1.83E-02	54.8	5.5	1.79E-02	2.23E-02	2.0	22.1
42	6.85E-03	146.1	2.1	6.08E-03	7.70E-03	11.2	12.4
43	2.04E-03	491.2	0.6	1.90E-03	2.45E-03	6.4	20.5
46	4.86E-01	2.1	145.8				
47	1.70E-01	5.9	51.0	1.45E-01	1.75E-01	14.8	2.9
48	1.35E-01	7.4	40.6	1.32E-01	1.60E-01	2.4	18.0
49	1.11E-01	9.0	33.2	1.03E-01	1.25E-01	6.9	13.0
50	5.54E-02	18.1	16.6	5.43E-02	6.65E-02	2.0	20.0
51	1.74E-02	57.4	5.2	1.86E-02	2.32E-02	6.9	33.0
52	1.06E-02	94.3	3.2	1.11E-02	1.39E-02	4.7	31.3
53	7.50E-03	133.3	2.3	6.75E-03	8.53E-03	10.0	13.7
54	6.73E-03	148.6	2.0	6.47E-03	8.18E-03	3.8	21.6
55	4.40E-03	227.4	1.3	3.79E-03	4.83E-03	13.8	9.9

Peak #	k_{exp} (h^{-1})	τ (h)	# τ in 300 h	k_{pred} Fixed T	k_{pred} Variable T	APE Fixed T	APE Variable T
56	5.05E-04	1980.2	0.2	7.54E-04	9.84E-04		
58	4.65E-02	21.5	14.0	5.03E-02	6.17E-02	8.2	32.7
59	3.70E-02	27.0	11.1	4.63E-02	5.69E-02	25.0	53.5
60	4.00E-02	25.0	12.0	4.22E-02	5.18E-02	5.5	29.7
61	3.19E-02	31.4	9.6	3.59E-02	4.42E-02	12.6	38.8
62	2.83E-02	35.3	8.5	2.94E-02	3.64E-02	3.8	28.4
63	2.53E-02	39.5	7.6	2.69E-02	3.33E-02	6.2	31.5
64	1.77E-02	56.5	5.3	1.95E-02	2.43E-02	10.2	37.1
65	1.69E-02	59.0	5.1	1.88E-02	2.34E-02	10.7	37.8
66	1.61E-02	62.1	4.8	1.67E-02	2.09E-02	4.0	29.6
67	1.09E-02	91.9	3.3	1.14E-02	1.42E-02	4.4	30.9
68	2.69E-02	37.2	8.1	2.42E-02	3.00E-02	10.0	11.6
69	1.49E-02	67.0	4.5	1.41E-02	1.77E-02	5.4	18.3
70	8.89E-03	112.5	2.7	8.19E-03	1.03E-02	7.9	16.0
71	8.44E-03	118.5	2.5	7.41E-03	9.35E-03	12.2	10.8
72	3.69E-03	271.4	1.1	3.08E-03	3.94E-03	16.4	6.9
73	2.64E-03	379.1	0.8	2.26E-03	2.91E-03	14.3	10.1
74	2.14E-03	468.1	0.6	1.74E-03	2.24E-03	18.6	4.9
75	1.27E-03	787.5	0.4	1.28E-03	1.65E-03		
76	9.00E-04	1111.0	0.3	1.01E-03	1.31E-03		
77	3.59E-04	2785.8	0.1	6.09E-04	7.98E-04		
78	7.85E-03	127.3	2.4	5.61E-03	7.11E-03	28.5	9.4

Table S4b. For model validation, the experimental rate constant (k_{exp}), characteristic lifetime (τ), and the number of τ in 300 h for selected compounds in diesel fuel evaporated at 20 °C. The predicted rate constant (k_{pred}) and absolute percent error (APE) were calculated using the fixed-temperature (Fixed T) and variable-temperature (Variable T) models. Compounds with τ < 0.5 in 300 h were excluded from the models (peaks 80, 85).

Peak #	k_{exp} (h^{-1})	τ (h)	# τ in 300 h	k_{pred} Fixed T	k_{pred} Variable T	APE Fixed T	APE Variable T
79	4.19E-03	238.7	1.3	4.45E-03	5.66E-03	6.2	35.0
81	7.50E-02	13.3	22.5	7.23E-02	8.82E-02	3.7	17.5
82	6.38E-03	156.7	1.9	6.40E-03	8.09E-03	0.3	26.9
83	6.22E-03	160.8	1.9	5.87E-03	7.43E-03	5.6	19.5
84	2.15E-03	465.9	0.6	1.98E-03	2.55E-03	7.7	18.8
86	2.44E-01	4.1	73.3	1.86E-01	2.24E-01	23.8	8.3
87	8.68E-02	11.5	26.0	7.97E-02	9.71E-02	8.2	11.9
88	7.63E-02	13.1	22.9	6.46E-02	7.90E-02	15.3	3.5
89	2.72E-02	36.7	8.2	2.96E-02	3.66E-02	8.6	34.3
90	2.81E-02	35.6	8.4	2.87E-02	3.55E-02	2.3	26.6
91	2.67E-02	37.5	8.0	2.56E-02	3.17E-02	4.0	19.0
92	1.01E-02	98.7	3.0	1.02E-02	1.28E-02	0.5	26.2
93	9.58E-03	104.4	2.9	9.04E-03	1.14E-02	5.6	18.8
94	2.36E-02	42.4	7.1	2.63E-02	3.26E-02	11.8	38.4
95	2.24E-02	44.6	6.7	2.55E-02	3.16E-02	13.8	41.0
96	1.81E-02	55.2	5.4	2.01E-02	2.50E-02	10.8	37.7
97	1.46E-02	68.3	4.4	1.81E-02	2.26E-02	23.8	54.1
98	1.24E-02	80.6	3.7	1.38E-02	1.73E-02	11.5	39.4
99	8.65E-03	115.5	2.6	9.56E-03	1.20E-02	10.5	38.9
100	7.20E-03	139.0	2.2	7.03E-03	8.87E-03	2.4	23.3
101	6.46E-03	154.7	1.9	6.21E-03	7.85E-03	4.0	21.5
102	5.93E-03	168.6	1.8	5.95E-03	7.53E-03	0.3	27.0
103	5.47E-03	182.9	1.6	5.43E-03	6.89E-03	0.6	26.0
104	8.69E-03	115.0	2.6	9.63E-03	1.21E-02	10.7	39.2
105	2.89E-03	345.9	0.9	2.93E-03	3.75E-03	1.3	29.6
106	2.72E-03	367.3	0.8	2.64E-03	3.39E-03	3.0	24.4
107	1.60E-02	62.6	4.8	1.73E-02	2.16E-02	8.6	35.3

Table S5a. For model development, the experimental rate constant (k_{exp}), characteristic lifetime (τ), and the number of τ in 300 h for selected compounds monitored during the evaporation of diesel fuel at 30 °C. The predicted rate constant (k_{pred}) and absolute percent error (APE) were calculated using the fixed-temperature (Fixed T) and variable-temperature (Variable T) models. Compounds with τ < 0.5 in 300 h were excluded from the models (peaks 24–37, 45, 77). Several compounds had retention indices lower than 800 (peaks 1, 38, 46) and were also excluded, as the retention index could not be accurately determined.

Peak #	k_{exp} (h^{-1})	τ (h)	# τ in 300 h	k_{pred} Fixed T	k_{pred} Variable T	APE Fixed T	APE Variable T
1	6.81E-01	1.5	204.2				
2	5.42E-01	1.8	162.5	4.40E-01	4.63E-01	18.8	14.5
3	2.26E-01	4.4	67.9	2.34E-01	2.46E-01	3.5	8.4
4	2.19E-01	4.6	65.8	2.17E-01	2.27E-01	1.2	3.4
5	1.62E-01	6.2	48.6	1.58E-01	1.65E-01	2.2	2.1
6	1.07E-01	9.3	32.2	1.13E-01	1.18E-01	5.3	9.7
7	1.04E-01	9.6	31.3	1.05E-01	1.10E-01	1.1	5.2
8	7.82E-02	12.8	23.4	8.57E-02	8.91E-02	9.7	14.0
9	7.17E-02	14.0	21.5	7.78E-02	8.08E-02	8.5	12.7
10	5.03E-02	19.9	15.1	5.70E-02	5.91E-02	13.3	17.4
11	3.99E-02	25.1	12.0	4.48E-02	4.63E-02	12.3	16.1
12	2.87E-02	34.8	8.6	3.17E-02	3.26E-02	10.3	13.7
13	2.51E-02	39.9	7.5	2.95E-02	3.04E-02	17.8	21.4
14	2.44E-02	41.1	7.3	2.77E-02	2.85E-02	13.7	17.1
15	1.84E-02	54.3	5.5	2.05E-02	2.11E-02	11.6	14.6
16	1.08E-02	92.5	3.2	1.17E-02	1.19E-02	7.9	10.3
17	9.87E-03	101.4	3.0	1.06E-02	1.08E-02	7.4	9.8
18	9.34E-03	107.0	2.8	9.92E-03	1.01E-02	6.2	8.5
19	6.21E-03	161.0	1.9	7.39E-03	7.53E-03	19.0	21.3
20	6.12E-03	163.3	1.8	6.26E-03	6.38E-03	2.3	4.1
21	4.38E-03	228.5	1.3	4.26E-03	4.33E-03	2.5	1.1
22	3.34E-03	299.8	1.0	3.39E-03	3.44E-03	1.8	3.1
23	2.24E-03	445.8	0.7	2.66E-03	2.69E-03	18.6	20.0
38	1.41E+00	0.7	423.4				
39	4.07E-01	2.5	122.2	3.32E-01	3.48E-01	18.6	14.5
40	1.39E-01	7.2	41.8	1.22E-01	1.28E-01	12.1	8.4
41	4.42E-02	22.6	13.3	4.32E-02	4.47E-02	2.2	1.1
42	1.54E-02	64.9	4.6	1.51E-02	1.54E-02	2.2	0.2
43	5.33E-03	187.8	1.6	4.84E-03	4.92E-03	9.1	7.7
44	1.89E-03	528.8	0.6	1.80E-03	1.82E-03	4.7	3.9
46	1.09E+00	0.9	325.8				
47	3.87E-01	2.6	116.1	3.34E-01	3.50E-01	13.8	9.5
48	3.09E-01	3.2	92.6	3.05E-01	3.20E-01	1.3	3.6
49	2.57E-01	3.9	77.2	2.40E-01	2.51E-01	6.9	2.5
50	1.37E-01	7.3	41.1	1.28E-01	1.33E-01	6.6	2.6
51	4.17E-02	24.0	12.5	4.50E-02	4.65E-02	7.7	11.4
52	2.53E-02	39.5	7.6	2.71E-02	2.79E-02	7.1	10.3
53	1.73E-02	57.8	5.2	1.67E-02	1.71E-02	3.7	1.2

Peak #	k_{exp} (h^{-1})	τ (h)	# τ in 300 h	k_{pred} Fixed T	k_{pred} Variable T	APE Fixed T	APE Variable T
54	1.51E-02	66.1	4.5	1.60E-02	1.64E-02	5.7	8.4
55	1.01E-02	99.5	3.0	9.49E-03	9.69E-03	5.6	3.6
56	1.92E-03	520.1	0.6	1.96E-03	1.97E-03	1.7	2.6
58	1.20E-01	8.3	36.1	1.19E-01	1.24E-01	1.2	3.0
59	9.14E-02	10.9	27.4	1.10E-01	1.14E-01	19.8	24.8
60	9.86E-02	10.1	29.6	9.99E-02	1.04E-01	1.3	5.4
61	7.99E-02	12.5	24.0	8.53E-02	8.87E-02	6.8	11.0
62	7.23E-02	13.8	21.7	7.03E-02	7.29E-02	2.7	0.9
63	6.12E-02	16.3	18.4	6.44E-02	6.67E-02	5.2	9.1
64	4.27E-02	23.4	12.8	4.71E-02	4.87E-02	10.1	13.9
65	4.08E-02	24.5	12.2	4.53E-02	4.68E-02	11.0	14.8
66	3.86E-02	25.9	11.6	4.05E-02	4.19E-02	4.9	8.4
67	2.48E-02	40.4	7.4	2.77E-02	2.86E-02	11.9	15.2
68	6.59E-02	15.2	19.8	5.81E-02	6.02E-02	11.8	8.6
69	3.55E-02	28.2	10.6	3.43E-02	3.54E-02	3.3	0.2
70	2.10E-02	47.6	6.3	2.01E-02	2.07E-02	4.2	1.6
71	1.96E-02	51.1	5.9	1.83E-02	1.87E-02	6.7	4.2
72	8.76E-03	114.2	2.6	7.74E-03	7.89E-03	11.6	9.9
73	6.85E-03	146.0	2.1	5.73E-03	5.82E-03	16.4	15.0
74	5.51E-03	181.4	1.7	4.43E-03	4.49E-03	19.7	18.5
75	3.90E-03	256.4	1.2	3.27E-03	3.32E-03	16.0	15.0
76	2.92E-03	342.5	0.9	2.60E-03	2.63E-03	11.1	10.1
78	1.67E-02	59.9	5.0	1.39E-02	1.43E-02	16.6	14.5

Table S5b. For model validation, the experimental rate constant (k_{exp}), characteristic lifetime (τ), and the number of τ in 300 h for selected compounds in diesel fuel evaporated at 30 °C. The predicted rate constant (k_{pred}) and absolute percent error (APE) were calculated using the fixed-temperature (Fixed T) and variable-temperature (Variable T) models. Compounds with τ < 0.5 in 300 h were excluded from the models.

Peak #	k_{exp} (h^{-1})	τ (h)	# τ in 300 h	k_{pred} Fixed T	k_{pred} Variable T	APE Fixed T	APE Variable T
79	1.03E-02	97.1	3.1	1.11E-02	1.13E-02	7.7	10.2
80	3.43E-03	291.2	1.0	3.57E-03	3.62E-03	4.1	5.5
81	1.75E-01	5.7	52.4	1.69E-01	1.77E-01	3.1	1.3
82	1.44E-02	69.4	4.3	1.58E-02	1.62E-02	9.9	12.7
83	1.45E-02	69.1	4.3	1.45E-02	1.49E-02	0.5	2.9
84	5.97E-03	167.6	1.8	5.03E-03	5.11E-03	15.7	14.3
85	2.75E-03	363.2	0.8	2.24E-03	2.26E-03	18.8	18.0
86	5.60E-01	1.8	168.0	4.27E-01	4.49E-01	23.8	19.8
87	1.98E-01	5.1	59.3	1.86E-01	1.95E-01	5.9	1.6
88	1.70E-01	5.9	51.0	1.52E-01	1.58E-01	10.9	7.0
89	6.70E-02	14.9	20.1	7.06E-02	7.33E-02	5.5	9.5
90	6.72E-02	14.9	20.1	6.87E-02	7.12E-02	2.2	6.0
91	6.24E-02	16.0	18.7	6.14E-02	6.36E-02	1.6	2.0
92	2.31E-02	43.3	6.9	2.49E-02	2.56E-02	7.7	10.8
93	2.22E-02	45.0	6.7	2.22E-02	2.28E-02	0.1	2.7
94	5.73E-02	17.5	17.2	6.31E-02	6.54E-02	10.1	14.1
95	5.38E-02	18.6	16.1	6.11E-02	6.33E-02	13.6	17.7
96	4.29E-02	23.3	12.9	4.84E-02	5.00E-02	12.6	16.5
97	3.54E-02	28.3	10.6	4.38E-02	4.52E-02	23.7	27.8
98	2.95E-02	33.9	8.8	3.36E-02	3.47E-02	14.2	17.8
99	1.99E-02	50.3	6.0	2.34E-02	2.41E-02	17.8	21.2
100	1.68E-02	59.7	5.0	1.73E-02	1.78E-02	3.4	6.1
101	1.45E-02	68.9	4.4	1.54E-02	1.57E-02	5.8	8.5
102	1.39E-02	71.8	4.2	1.47E-02	1.51E-02	5.8	8.5
103	1.27E-02	78.5	3.8	1.35E-02	1.38E-02	5.8	8.4
104	1.95E-02	51.3	5.8	2.36E-02	2.43E-02	21.0	24.5
105	7.39E-03	135.3	2.2	7.37E-03	7.51E-03	0.3	1.6
106	7.26E-03	137.7	2.2	6.66E-03	6.79E-03	8.2	6.6
107	3.92E-02	25.5	11.8	4.19E-02	4.33E-02	6.8	10.4

Table S6a. For model development, the experimental rate constant (k_{exp}), characteristic lifetime (τ), and the number of τ in 300 h for selected compounds monitored during the evaporation of diesel fuel at 35 °C. The predicted rate constant (k_{pred}) and absolute percent error (APE) were calculated using the fixed-temperature (Fixed T) and variable-temperature (Variable T) models. Compounds with τ < 0.5 in 300 h were excluded from the models (peaks 26–37, 45). Several compounds had retention indices lower than 800 (peaks 1, 38, 46) and were also excluded, as the retention index could not be accurately determined.

Peak #	k_{exp} (h^{-1})	τ (h)	# τ in 300 h	k_{pred} Fixed T	k_{pred} Variable T	APE Fixed T	APE Variable T
1	1.44E+00	0.7	432.4				
2	1.00E+00	1.0	300.0	6.82E-01	6.46E-01	31.8	35.4
3	3.95E-01	2.5	118.5	3.68E-01	3.43E-01	6.8	13.3
4	3.79E-01	2.6	113.8	3.41E-01	3.16E-01	10.1	16.6
5	2.54E-01	3.9	76.1	2.51E-01	2.31E-01	1.2	9.1
6	1.75E-01	5.7	52.6	1.80E-01	1.64E-01	2.8	6.3
7	1.69E-01	5.9	50.7	1.68E-01	1.53E-01	0.4	9.5
8	1.26E-01	7.9	37.9	1.37E-01	1.24E-01	8.7	1.7
9	1.11E-01	9.0	33.3	1.25E-01	1.13E-01	12.4	1.4
10	7.66E-02	13.0	23.0	9.22E-02	8.24E-02	20.2	7.5
11	6.34E-02	15.8	19.0	7.28E-02	6.46E-02	14.8	1.9
12	4.68E-02	21.3	14.1	5.18E-02	4.55E-02	10.6	2.8
13	4.20E-02	23.8	12.6	4.84E-02	4.24E-02	15.3	1.1
14	4.04E-02	24.8	12.1	4.54E-02	3.98E-02	12.5	1.5
15	2.89E-02	34.6	8.7	3.39E-02	2.94E-02	17.2	1.8
16	1.82E-02	54.9	5.5	1.95E-02	1.66E-02	6.9	8.6
17	1.61E-02	62.2	4.8	1.77E-02	1.51E-02	10.3	6.0
18	1.52E-02	65.9	4.6	1.66E-02	1.41E-02	9.6	6.8
19	1.10E-02	90.5	3.3	1.25E-02	1.05E-02	12.8	4.9
20	9.98E-03	100.2	3.0	1.06E-02	8.89E-03	6.2	10.9
21	7.28E-03	137.5	2.2	7.27E-03	6.04E-03	0.1	17.0
22	5.87E-03	170.4	1.8	5.81E-03	4.80E-03	0.9	18.3
23	4.04E-03	247.7	1.2	4.58E-03	3.75E-03	13.4	7.0
24	2.41E-03	414.2	0.7	2.39E-03	1.92E-03	1.0	20.4
25	2.16E-03	463.4	0.6	2.07E-03	1.66E-03	4.2	23.3
38	2.86E+00	0.3	858.6				
39	7.52E-01	1.3	225.6	5.17E-01	4.86E-01	31.2	35.4
40	2.14E-01	4.7	64.1	1.95E-01	1.78E-01	8.7	16.6
41	6.86E-02	14.6	20.6	7.03E-02	6.23E-02	2.4	9.2
42	2.55E-02	39.3	7.6	2.50E-02	2.15E-02	1.8	15.5
43	8.69E-03	115.1	2.6	8.23E-03	6.86E-03	5.3	21.1
44	3.91E-03	255.7	1.2	3.13E-03	2.53E-03	20.1	35.2
46	2.13E+00	0.5	637.9				
47	6.74E-01	1.5	202.1	5.20E-01	4.89E-01	22.8	27.5
48	5.46E-01	1.8	163.7	4.76E-01	4.46E-01	12.7	18.2
49	4.34E-01	2.3	130.1	3.76E-01	3.50E-01	13.3	19.3
50	2.11E-01	4.7	63.2	2.03E-01	1.86E-01	3.4	11.7
51	6.43E-02	15.5	19.3	7.31E-02	6.49E-02	13.6	0.8

Peak #	k_{exp} (h^{-1})	τ (h)	# τ in 300 h	k_{pred} Fixed T	k_{pred} Variable T	APE Fixed T	APE Variable T
52	3.95E-02	25.3	11.8	4.45E-02	3.89E-02	12.7	1.4
53	2.75E-02	36.3	8.3	2.76E-02	2.39E-02	0.4	13.4
54	2.50E-02	40.0	7.5	2.65E-02	2.29E-02	6.2	8.5
55	1.64E-02	60.9	4.9	1.59E-02	1.35E-02	3.1	17.7
56	3.84E-03	260.6	1.2	3.39E-03	2.75E-03	11.7	28.3
58	1.75E-01	5.7	52.6	1.89E-01	1.73E-01	7.9	1.5
59	1.42E-01	7.1	42.5	1.75E-01	1.59E-01	23.4	12.4
60	1.49E-01	6.7	44.7	1.60E-01	1.45E-01	7.1	2.7
61	1.18E-01	8.5	35.3	1.37E-01	1.24E-01	16.2	5.0
62	1.06E-01	9.5	31.7	1.13E-01	1.02E-01	7.2	3.6
63	9.04E-02	11.1	27.1	1.04E-01	9.31E-02	14.9	3.0
64	6.49E-02	15.4	19.5	7.64E-02	6.79E-02	17.7	4.6
65	6.30E-02	15.9	18.9	7.35E-02	6.53E-02	16.7	3.6
66	5.94E-02	16.8	17.8	6.60E-02	5.84E-02	11.1	1.7
67	4.03E-02	24.8	12.1	4.55E-02	3.98E-02	12.7	1.3
68	1.01E-01	9.9	30.3	9.39E-02	8.40E-02	7.0	16.9
69	5.42E-02	18.4	16.3	5.61E-02	4.94E-02	3.4	8.9
70	3.32E-02	30.1	10.0	3.32E-02	2.88E-02	0.0	13.2
71	3.06E-02	32.7	9.2	3.02E-02	2.61E-02	1.2	14.5
72	1.45E-02	68.8	4.4	1.30E-02	1.10E-02	10.3	24.2
73	1.09E-02	91.9	3.3	9.70E-03	8.12E-03	10.8	25.3
74	8.71E-03	114.7	2.6	7.54E-03	6.27E-03	13.5	28.1
75	6.42E-03	155.7	1.9	5.61E-03	4.63E-03	12.6	28.0
76	5.19E-03	192.8	1.6	4.47E-03	3.66E-03	13.8	29.4
77	3.34E-03	299.2	1.0	2.76E-03	2.23E-03	17.3	33.3
78	2.82E-02	35.4	8.5	2.32E-02	1.99E-02	17.9	29.5

Table S6b. For model validation, the experimental rate constant (k_{exp}), characteristic lifetime (τ), and the number of τ in 300 h for selected compounds in diesel fuel evaporated at 35 °C. The predicted rate constant (k_{pred}) and absolute percent error (APE) were calculated using the fixed-temperature (Fixed T) and variable-temperature (Variable T) models. Compounds with τ < 0.5 in 300 h were excluded from the models.

Peak #	k_{exp} (h^{-1})	τ (h)	# τ in 300 h	k_{pred} Fixed T	k_{pred} Variable T	APE Fixed T	APE Variable T
79	1.73E-02	57.9	5.2	1.85E-02	1.58E-02	7.3	8.5
80	6.10E-03	163.9	1.8	6.11E-03	5.05E-03	0.2	17.2
81	2.92E-01	3.4	87.7	2.68E-01	2.47E-01	8.5	15.7
82	2.43E-02	41.1	7.3	2.63E-02	2.26E-02	7.9	7.0
83	2.35E-02	42.5	7.1	2.42E-02	2.08E-02	2.8	11.6
84	9.24E-03	108.2	2.8	8.54E-03	7.13E-03	7.6	22.9
85	4.86E-03	205.7	1.5	3.86E-03	3.15E-03	20.6	35.3
86	1.06E+00	0.9	317.7	6.62E-01	6.26E-01	37.5	40.9
87	3.10E-01	3.2	93.0	2.94E-01	2.71E-01	5.3	12.4
88	2.74E-01	3.7	82.2	2.40E-01	2.21E-01	12.3	19.4
89	1.05E-01	9.5	31.4	1.14E-01	1.02E-01	8.5	2.4
90	1.05E-01	9.5	31.5	1.11E-01	9.93E-02	5.2	5.5
91	9.82E-02	10.2	29.5	9.91E-02	8.87E-02	0.9	9.7
92	3.84E-02	26.0	11.5	4.09E-02	3.57E-02	6.6	7.0
93	3.65E-02	27.4	10.9	3.65E-02	3.18E-02	0.2	12.8
94	8.99E-02	11.1	27.0	1.02E-01	9.12E-02	13.2	1.4
95	8.43E-02	11.9	25.3	9.86E-02	8.83E-02	17.0	4.8
96	6.57E-02	15.2	19.7	7.84E-02	6.98E-02	19.4	6.2
97	5.60E-02	17.8	16.8	7.11E-02	6.31E-02	27.0	12.6
98	4.71E-02	21.2	14.1	5.50E-02	4.84E-02	16.8	2.8
99	3.22E-02	31.0	9.7	3.86E-02	3.36E-02	19.6	4.2
100	2.70E-02	37.0	8.1	2.87E-02	2.48E-02	6.2	8.2
101	2.46E-02	40.7	7.4	2.55E-02	2.20E-02	3.7	10.7
102	2.27E-02	44.0	6.8	2.45E-02	2.11E-02	7.7	7.4
103	2.07E-02	48.2	6.2	2.24E-02	1.93E-02	8.2	7.1
104	3.23E-02	31.0	9.7	3.88E-02	3.38E-02	20.4	4.9
105	1.16E-02	86.4	3.5	1.24E-02	1.05E-02	7.3	9.5
106	1.13E-02	88.9	3.4	1.13E-02	9.47E-03	0.0	15.9
107	5.87E-02	17.0	17.6	6.82E-02	6.04E-02	16.1	2.9