

# Supporting Information for Modeling the Formation and Composition of Secondary Organic Aerosol from Diesel Exhaust Using Parameterized and Semi-explicit Chemistry and Thermodynamic Models

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Table S1: Mass speciation and  $k_{OH}$  for VOC emissions profile #3161

Species Name	$k_{OH}$ ( $\text{cm}^3 \text{ molecules}^{-1} \text{ s}^{-1}$ )	Mass Percent (%)
(1-methylpropyl) benzene	$8.50 \times 10^{-12}$	0.023
(2-methylpropyl) benzene	$8.71 \times 10^{-12}$	0.060
1,2,3-trimethylbenzene	$3.27 \times 10^{-11}$	0.056
1,2,4-trimethylbenzene	$3.25 \times 10^{-11}$	0.246
1,2-diethylbenzene	$8.11 \times 10^{-12}$	0.042
1,2-propadiene	$9.82 \times 10^{-12}$	0.218
1,3,5-trimethylbenzene	$5.67 \times 10^{-11}$	0.088
1,3-butadiene	$6.66 \times 10^{-11}$	0.088
1-butene	$3.14 \times 10^{-11}$	0.311
1-methyl-2-ethylbenzene	$7.44 \times 10^{-12}$	0.065
1-methyl-3-ethylbenzene	$1.39 \times 10^{-11}$	0.116
1-pentene	$3.14 \times 10^{-11}$	0.148
2,2,4-trimethylpentane	$3.34 \times 10^{-12}$	0.139
2,2-dimethylbutane	$2.23 \times 10^{-12}$	0.028
2,3,4-trimethylpentane	$6.60 \times 10^{-12}$	0.009
2,3-dimethyl-1-butene	$5.38 \times 10^{-11}$	0.014
2,3-dimethylhexane	$8.55 \times 10^{-12}$	0.005
2,3-dimethylpentane	$7.14 \times 10^{-12}$	0.032
2,4-dimethylhexane	$8.55 \times 10^{-12}$	0.019
2,4-dimethylpentane	$4.77 \times 10^{-12}$	0.009
2-methylheptane	$8.28 \times 10^{-12}$	0.028
2-methylhexane	$6.86 \times 10^{-12}$	0.056
2-methylpentane	$5.20 \times 10^{-12}$	0.181
3,3-dimethyl-1-butene	$2.80 \times 10^{-11}$	1.308
3-ethylhexane	$8.97 \times 10^{-12}$	0.028
3-methylhexane	$7.15 \times 10^{-12}$	0.162
3-methylpentane	$5.20 \times 10^{-12}$	0.056
acetaldehyde	$1.50 \times 10^{-11}$	3.409
acetone	$1.70 \times 10^{-13}$	3.483
acetylene	$8.15 \times 10^{-13}$	1.971
alkene ketone	$1.70 \times 10^{-13}$	0.812
b-methylstyrene	$3.12 \times 10^{-11}$	0.023
benzaldehyde	$1.20 \times 10^{-11}$	0.325
benzene	$1.22 \times 10^{-12}$	0.928
butyraldehyde	$2.40 \times 10^{-11}$	0.867
c10 aromatics	$2.30 \times 10^{-11}$	0.037
c5 aldehyde	$2.88 \times 10^{-11}$	0.051
c6 aldehydes	$2.88 \times 10^{-11}$	1.763
c9 aromatics	$2.31 \times 10^{-11}$	0.232
cis-2-butene	$5.64 \times 10^{-11}$	0.042

cis-2-pentene	$6.50 \times 10^{-11}$	0.014
cyclohexane	$6.97 \times 10^{-12}$	0.014
cyclohexanone	$6.40 \times 10^{-12}$	0.051
cyclopentane	$4.97 \times 10^{-12}$	0.005
ethane	$2.48 \times 10^{-13}$	0.264
ethyl alcohol	$3.58 \times 10^{-12}$	0.005
ethylbenzene	$7.00 \times 10^{-12}$	0.144
ethylene	$8.52 \times 10^{-12}$	6.670
formaldehyde	$9.37 \times 10^{-12}$	6.823
indan	$1.90 \times 10^{-11}$	0.088
isobutane	$2.44 \times 10^{-12}$	0.566
isobutylene	$5.14 \times 10^{-11}$	0.427
butylbenzene	$4.50 \times 10^{-12}$	0.060
diethylbenzene	$8.11 \times 10^{-12}$	0.065
isopentane	$3.60 \times 10^{-12}$	0.278
isopropylbenzene	$6.90 \times 10^{-12}$	0.009
<i>m</i> -xylene	$2.31 \times 10^{-11}$	0.283
methane	$6.4 \times 10^{-15}$	1.892
methyl alcohol	$6.16 \times 10^{-13}$	0.014
methyl ethyl ketone	$1.22 \times 10^{-12}$	0.686
2-hexanone	$9.10 \times 10^{-12}$	0.417
methylcyclohexane	$9.64 \times 10^{-12}$	0.032
methylcyclopentane	$5.66 \times 10^{-12}$	0.070
<i>n</i> -butane	$2.36 \times 10^{-12}$	0.046
<i>n</i> -decane	$1.10 \times 10^{-11}$	0.246
<i>n</i> -heptane	$6.76 \times 10^{-12}$	0.032
<i>n</i> -hexane	$5.20 \times 10^{-12}$	0.074
<i>n</i> -nonane	$9.70 \times 10^{-12}$	0.107
<i>n</i> -octane	$8.11 \times 10^{-12}$	0.065
<i>n</i> -pentane	$3.80 \times 10^{-12}$	0.083
<i>n</i> -propylbenzene	$5.8 \times 10^{-12}$	0.056
<i>n</i> -undecane	$1.23 \times 10^{-11}$	0.121
naphthalene	$2.30 \times 10^{-11}$	0.042
<i>o</i> -xylene	$1.36 \times 10^{-11}$	0.158
<i>p</i> -xylene	$1.43 \times 10^{-11}$	0.046
propane	$1.09 \times 10^{-12}$	0.088
propionaldehyde	$2.20 \times 10^{-11}$	0.450
propylene	$2.64 \times 10^{-11}$	1.206
styrene	$5.80 \times 10^{-11}$	0.028
<i>t</i> -butylbenzene	$4.50 \times 10^{-12}$	0.005
unknown	$1.23 \times 10^{-11}$	0.093
trans-2-butene	$6.40 \times 10^{-11}$	0.019
trans-2-pentene	$6.70 \times 10^{-11}$	0.682
toluene	$5.63 \times 10^{-12}$	2.268
C <sub>12</sub> branched alkane	$1.82 \times 10^{-11}$	1.623
C <sub>13</sub> branched alkane	$1.68 \times 10^{-11}$	1.052
C <sub>14</sub> branched alkane	$1.39 \times 10^{-11}$	0.939
C <sub>15</sub> branched alkane	$1.82 \times 10^{-11}$	0.988
C <sub>16</sub> branched alkane	$1.96 \times 10^{-11}$	0.440
C <sub>17</sub> branched alkane	$2.1 \times 10^{-11}$	0.573
C <sub>18</sub> branched alkane	$2.24 \times 10^{-11}$	0.343
C <sub>19</sub> branched alkane	$2.38 \times 10^{-11}$	0.194
C <sub>20</sub> branched alkane	$2.52 \times 10^{-11}$	0.128
C <sub>21</sub> branched alkane	$2.67 \times 10^{-11}$	0.121
C <sub>22</sub> branched alkane	$2.81 \times 10^{-11}$	8.690
C <sub>12</sub> cyclic alkane	$1.82 \times 10^{-11}$	8.858

C <sub>13</sub> cyclic alkane	1.68×10 <sup>-11</sup>	6.299
C <sub>14</sub> cyclic alkane	1.39×10 <sup>-11</sup>	5.723
C <sub>15</sub> cyclic alkane	1.82×10 <sup>-11</sup>	4.372
C <sub>16</sub> cyclic alkane	1.96×10 <sup>-11</sup>	3.711
C <sub>17</sub> cyclic alkane	2.1×10 <sup>-11</sup>	3.382
C <sub>18</sub> cyclic alkane	2.24×10 <sup>-11</sup>	2.115
C <sub>19</sub> cyclic alkane	2.38×10 <sup>-11</sup>	1.181
C <sub>20</sub> cyclic alkane	2.52×10 <sup>-11</sup>	0.748
C <sub>21</sub> cyclic alkane	2.67×10 <sup>-11</sup>	0.629
C <sub>22</sub> cyclic alkane	2.81×10 <sup>-11</sup>	1.167
<i>n</i> -dodecane	1.82×10 <sup>-11</sup>	1.094
<i>n</i> -tridecane	1.68×10 <sup>-11</sup>	0.730
<i>n</i> -tetradecane	1.39×10 <sup>-11</sup>	0.613
<i>n</i> -pentadecane	1.82×10 <sup>-11</sup>	0.456
<i>n</i> -hexadecane	1.96×10 <sup>-11</sup>	0.331
<i>n</i> -heptadecane	2.1×10 <sup>-11</sup>	0.296
<i>n</i> -octadecane	2.24×10 <sup>-11</sup>	0.145
<i>n</i> -nonadecane	2.38×10 <sup>-11</sup>	0.073
<i>n</i> -eicosane	2.52×10 <sup>-11</sup>	0.044
<i>n</i> -heneicosane	2.67×10 <sup>-11</sup>	0.029
<i>n</i> -docosane	2.81×10 <sup>-11</sup>	0.287
pristane	2.44×10 <sup>-11</sup>	0.160
phytane	2.61×10 <sup>-11</sup>	0.208
naphthalene	2.3×10 <sup>-11</sup>	0.023
phenanthrene	1.3×10 <sup>-11</sup>	0.023

Table S2: Mass speciation and  $k_{OH}$  for VOC emissions profile #8774

<i>Species Name</i>	$k_{OH}$ (cm <sup>3</sup> molecules <sup>-1</sup> s <sup>-1</sup> )	Mass Percent (%)
1,2,3,5-tetramethylbenzene	4.30×10 <sup>-10</sup>	0.069
1,2,3-trimethylbenzene	3.27×10 <sup>-10</sup>	0.050
1,2,4,5-tetramethylbenzene	2.05×10 <sup>-10</sup>	0.033
1,2,4-trimethylbenzene	3.25×10 <sup>-10</sup>	0.021
1,2-butadiene	6.66×10 <sup>-10</sup>	0.010
1,3,5-trimethylbenzene	5.67×10 <sup>-10</sup>	0.042
1,3-butadiene	6.66×10 <sup>-10</sup>	0.344
1,3-diethylbenzene	1.42×10 <sup>-10</sup>	0.068
1,3-hexadiene	1.06×10 <sup>-09</sup>	0.015
1,4-diethylbenzene	8.10×10 <sup>-11</sup>	0.091
1-butene	3.14×10 <sup>-10</sup>	0.872
1-heptene	3.15×10 <sup>-10</sup>	0.152
1-methyl-2-ethylbenzene	7.43×10 <sup>-11</sup>	0.078
1-methyl-3-ethylbenzene	1.38×10 <sup>-10</sup>	0.047
1-methyl-4-ethylbenzene	7.43×10 <sup>-11</sup>	0.039
1-methylindan	9.16×10 <sup>-11</sup>	0.028
1-pentene	3.14×10 <sup>-10</sup>	0.183
1-propyne	7.13×10 <sup>-11</sup>	0.089
2,2,4-trimethylpentane	3.34×10 <sup>-11</sup>	0.262
2,2,5-trimethylhexane	6.04×10 <sup>-11</sup>	0.057
2,2-dimethylbutane	1.89×10 <sup>-11</sup>	0.043
2,3,4-trimethylpentane	6.60×10 <sup>-11</sup>	0.032
2,3-dimethyl-2-pentene	1.11×10 <sup>-09</sup>	0.002
2,3-dimethylbutane	5.44×10 <sup>-11</sup>	0.067
2,3-dimethylhexane	8.55×10 <sup>-11</sup>	0.007
2,3-dimethylpentane	7.13×10 <sup>-11</sup>	0.078
2,4-dimethylpentane	4.77×10 <sup>-11</sup>	0.243
2,6-dimethylheptane	9.68×10 <sup>-11</sup>	0.000

2-methyl-1-butene	$5.26 \times 10^{-10}$	0.103
2-methyl-1-pentene	$5.40 \times 10^{-10}$	2.833
2-methyl-2-butene	$8.73 \times 10^{-10}$	0.117
2-methyl-2-pentene	$8.82 \times 10^{-10}$	0.012
2-methylheptane	$8.27 \times 10^{-11}$	0.062
2-methylhexane	$6.86 \times 10^{-11}$	0.070
2-methylindan	$9.41 \times 10^{-11}$	0.017
2-methylpentane	$5.20 \times 10^{-11}$	0.039
3-methyl-cis-2-pentene	$8.82 \times 10^{-10}$	0.009
3-methyl-trans-2-pentene	$8.82 \times 10^{-10}$	0.111
3-methylheptane	$8.56 \times 10^{-11}$	0.054
3-methylhexane	$7.14 \times 10^{-11}$	0.130
3-methyloctane	$9.97 \times 10^{-11}$	0.142
4-methylheptane	$8.27 \times 10^{-11}$	0.018
acetaldehyde	$1.50 \times 10^{-10}$	2.228
acetylene	$8.15 \times 10^{-12}$	2.675
alpha-pinene	$9.07 \times 10^{-10}$	0.035
benzaldehyde	$1.20 \times 10^{-10}$	0.231
benzene	$1.22 \times 10^{-11}$	1.281
beta-pinene	$5.65 \times 10^{-10}$	0.001
butyraldehyde	$2.40 \times 10^{-10}$	0.514
cis-2-butene	$5.64 \times 10^{-10}$	0.098
cis-2-hexene	$5.90 \times 10^{-10}$	0.021
cis-2-pentene	$6.50 \times 10^{-10}$	0.053
crotonaldehyde	$3.61 \times 10^{-10}$	0.128
cyclohexane	$6.97 \times 10^{-11}$	0.120
cyclohexene	$6.15 \times 10^{-10}$	0.051
cyclopentane	$4.97 \times 10^{-11}$	0.038
cyclopentene	$5.87 \times 10^{-10}$	0.060
dl-limonene	$1.45 \times 10^{-09}$	0.012
ethane	$2.48 \times 10^{-12}$	0.739
ethylbenzene	$7.00 \times 10^{-11}$	0.147
ethylene	$8.52 \times 10^{-11}$	8.180
formaldehyde	$9.37 \times 10^{-11}$	3.554
glyoxal	$2.53 \times 10^{-10}$	0.296
indan	$8.27 \times 10^{-11}$	0.028
isobutane	$2.44 \times 10^{-11}$	0.305
isopentane	$3.60 \times 10^{-11}$	1.721
isoprene	$1.05 \times 10^{-09}$	0.061
isopropylbenzene	$6.90 \times 10^{-11}$	0.013
isopropylcyclohexane	$1.33 \times 10^{-10}$	0.150
isopropyltoluene	$8.53 \times 10^{-11}$	0.062
<i>m</i> & <i>p</i> -xylene	$2.31 \times 10^{-10}$	0.252
2-butanone	$1.22 \times 10^{-11}$	1.198
methylcyclohexane	$9.64 \times 10^{-11}$	0.115
methylcyclopentane	$5.66 \times 10^{-11}$	1.786
<i>n</i> -butane	$2.36 \times 10^{-11}$	0.573
<i>n</i> -butylbenzene	$8.72 \times 10^{-11}$	0.021
<i>n</i> -decane	$1.10 \times 10^{-10}$	0.404
<i>n</i> -heptane	$6.76 \times 10^{-11}$	0.125
<i>n</i> -hexane	$5.20 \times 10^{-11}$	0.307
<i>n</i> -nonane	$9.70 \times 10^{-11}$	0.159
<i>n</i> -octane	$8.11 \times 10^{-11}$	0.145
<i>n</i> -pentane	$3.80 \times 10^{-11}$	0.313
<i>n</i> -propylbenzene	$5.80 \times 10^{-11}$	0.026
<i>n</i> -undecane	$1.23 \times 10^{-10}$	0.417

<i>o</i> -xylene	$1.36 \times 10^{-10}$	0.104
<i>n</i> -propane	$1.09 \times 10^{-11}$	0.890
propionaldehyde	$2.19 \times 10^{-10}$	0.257
propylene	$2.64 \times 10^{-10}$	2.347
propyltoluene	$8.80 \times 10^{-11}$	0.050
styrene	$5.80 \times 10^{-10}$	0.129
tolualdehyde	$1.86 \times 10^{-10}$	0.016
toluene	$5.63 \times 10^{-12}$	0.588
trans-1,3-dichloropropene	$9.35 \times 10^{-11}$	0.002
trans-2-butene	$6.40 \times 10^{-10}$	0.121
trans-2-hexene	$6.66 \times 10^{-10}$	0.036
trans-2-pentene	$6.7 \times 10^{-10}$	0.054
valeraldehyde	$2.74 \times 10^{-10}$	0.023
C <sub>12</sub> branched alkane	$1.82 \times 10^{-11}$	1.623
C <sub>13</sub> branched alkane	$1.68 \times 10^{-11}$	1.052
C <sub>14</sub> branched alkane	$1.39 \times 10^{-11}$	0.939
C <sub>15</sub> branched alkane	$1.82 \times 10^{-11}$	0.988
C <sub>16</sub> branched alkane	$1.96 \times 10^{-11}$	0.440
C <sub>17</sub> branched alkane	$2.1 \times 10^{-11}$	0.573
C <sub>18</sub> branched alkane	$2.24 \times 10^{-11}$	0.343
C <sub>19</sub> branched alkane	$2.38 \times 10^{-11}$	0.194
C <sub>20</sub> branched alkane	$2.52 \times 10^{-11}$	0.128
C <sub>21</sub> branched alkane	$2.67 \times 10^{-11}$	0.121
C <sub>22</sub> branched alkane	$2.81 \times 10^{-11}$	8.690
C <sub>12</sub> cyclic alkane	$1.82 \times 10^{-11}$	8.858
C <sub>13</sub> cyclic alkane	$1.68 \times 10^{-11}$	6.299
C <sub>14</sub> cyclic alkane	$1.39 \times 10^{-11}$	5.723
C <sub>15</sub> cyclic alkane	$1.82 \times 10^{-11}$	4.372
C <sub>16</sub> cyclic alkane	$1.96 \times 10^{-11}$	3.711
C <sub>17</sub> cyclic alkane	$2.1 \times 10^{-11}$	3.382
C <sub>18</sub> cyclic alkane	$2.24 \times 10^{-11}$	2.115
C <sub>19</sub> cyclic alkane	$2.38 \times 10^{-11}$	1.181
C <sub>20</sub> cyclic alkane	$2.52 \times 10^{-11}$	0.748
C <sub>21</sub> cyclic alkane	$2.67 \times 10^{-11}$	0.629
C <sub>22</sub> cyclic alkane	$2.81 \times 10^{-11}$	1.167
<i>n</i> -dodecane	$1.82 \times 10^{-11}$	1.094
<i>n</i> -tridecane	$1.68 \times 10^{-11}$	0.730
<i>n</i> -tetradecane	$1.39 \times 10^{-11}$	0.613
<i>n</i> -pentadecane	$1.82 \times 10^{-11}$	0.456
<i>n</i> -hexadecane	$1.96 \times 10^{-11}$	0.331
<i>n</i> -heptadecane	$2.1 \times 10^{-11}$	0.296
<i>n</i> -octadecane	$2.24 \times 10^{-11}$	0.145
<i>n</i> -nonadecane	$2.38 \times 10^{-11}$	0.073
<i>n</i> -eicosane	$2.52 \times 10^{-11}$	0.044
<i>n</i> -heneicosane	$2.67 \times 10^{-11}$	0.029
<i>n</i> -docosane	$2.81 \times 10^{-11}$	0.287
pristane	$2.44 \times 10^{-11}$	0.160
phytane	$2.61 \times 10^{-11}$	0.208
naphthalene	$2.30 \times 10^{-11}$	0.023
phenanthrene	$1.30 \times 10^{-11}$	0.023

Table S3: Mass speciation and  $k_{OH}$  for VOC emissions profile #4777

Species Name	$k_{OH}$ ( $\text{cm}^3 \text{molecules}^{-1} \text{s}^{-1}$ )	Mass Percent (%)
1,1,4-trimethylcyclohexane	$9.09 \times 10^{-12}$	0.081
1,2,4-trimethylbenzene	$1.67 \times 10^{-11}$	0.405
1,2-dimethyl-4-ethylbenzene	$1.69 \times 10^{-11}$	0.177

1,3,5-trimethylbenzene	$3.51 \times 10^{-11}$	0.162
1,3-dimethyl-2-ethylbenzene	$1.76 \times 10^{-11}$	0.283
1,4-dimethyl-2-ethylbenzene	$1.69 \times 10^{-11}$	0.374
1-(1,1-dimethylethyl)-3,5-dimethylbenzene	$3.01 \times 10^{-11}$	0.319
1-butene	$3.14 \times 10^{-11}$	0.521
1-ethyl-1-methylcyclopentane	$6.33 \times 10^{-12}$	0.035
1-hexene	$3.02 \times 10^{-11}$	0.152
1-methyl-2-ethylbenzene	$7.44 \times 10^{-12}$	0.329
1-methyl-2-tert-butylbenzene	$6.74 \times 10^{-12}$	0.369
1-methyl-3-ethylbenzene	$1.39 \times 10^{-11}$	0.617
1-methyl-3-isopropylbenzene	$1.45 \times 10^{-11}$	0.379
1-methyl-3-propylbenzene	$1.52 \times 10^{-11}$	0.233
1-methyl-4-ethylbenzene	$7.44 \times 10^{-12}$	0.182
1-nonene	$3.44 \times 10^{-11}$	0.061
1-pentene	$3.14 \times 10^{-11}$	0.273
1-tert-butyl-4-ethylbenzene	$7.42 \times 10^{-12}$	0.167
2,2,4-trimethylpentane	$3.16 \times 10^{-11}$	0.197
2,2-dimethylbutane	$1.82 \times 10^{-12}$	0.101
2,2-dimethylpropane	$6.69 \times 10^{-13}$	0.051
2,3,4-trimethylpentane	$8.54 \times 10^{-12}$	0.046
2,3-dimethylbutane	$5.44 \times 10^{-12}$	0.020
2,3-dimethylhexane	$5.09 \times 10^{-12}$	0.106
2,3-dimethylpentane	$7.14 \times 10^{-12}$	0.015
2,4-dimethylhexane	$4.92 \times 10^{-12}$	0.051
2,4-dimethylpentane	$6.85 \times 10^{-12}$	0.010
2,5-dimethylheptane	$9.97 \times 10^{-12}$	0.071
2,5-dimethylhexane	$7.24 \times 10^{-12}$	0.025
2-methyl-butyl-benzene	$1.02 \times 10^{-11}$	0.946
2-methylhexane	$6.86 \times 10^{-12}$	0.293
2-methylnonane	$1.11 \times 10^{-11}$	0.273
2-methyloctane	$9.97 \times 10^{-12}$	0.091
2-methylpentane	$5.45 \times 10^{-12}$	0.040
3,3-dimethyloctane	$7.21 \times 10^{-12}$	0.263
3,3-dimethylpentane	$2.97 \times 10^{-12}$	0.081
3,5-dimethylheptane	$1.02 \times 10^{-11}$	0.076
3-ethyloctane	$1.18 \times 10^{-11}$	0.162
3-ethylpentane	$7.56 \times 10^{-12}$	0.030
3-methyl-1-butene	$2.86 \times 10^{-11}$	0.111
3-methyl-cis-2-pentene	$8.83 \times 10^{-11}$	0.071
3-methylheptane	$8.56 \times 10^{-12}$	0.056
3-methylhexane	$7.15 \times 10^{-12}$	0.020
3-methylnonane	$1.14 \times 10^{-11}$	0.228
3-methylpentane	$5.73 \times 10^{-12}$	0.071
4-methyl-1-pentene	$3.02 \times 10^{-11}$	0.061
4-methylheptane	$1.02 \times 10^{-11}$	0.475
acetaldehyde	$1.50 \times 10^{-11}$	2.710
acetone	$1.70 \times 10^{-13}$	3.828
acetylene	$8.15 \times 10^{-13}$	2.346
acrolein	$2.58 \times 10^{-11}$	0.759
benzene	$1.22 \times 10^{-12}$	1.370
cis,trans-1,2,4-trimethylcyclohexane	$1.35 \times 10^{-11}$	3.580
cis-2-butene	$5.64 \times 10^{-11}$	0.056
cis-2-nonene	$6.32 \times 10^{-11}$	0.096
cis-2-octene	$6.18 \times 10^{-11}$	0.046
cis-3-hexene	$2.00 \times 10^{-10}$	0.066
crotonaldehyde	$3.62 \times 10^{-11}$	0.228

cyclohexane	$6.97 \times 10^{-12}$	0.015
cyclohexane	$6.97 \times 10^{-12}$	0.071
cyclopentane	$4.97 \times 10^{-12}$	0.030
cyclopentene	$5.88 \times 10^{-11}$	0.046
ethane	$2.48 \times 10^{-13}$	0.172
ethylbenzene	$7.00 \times 10^{-12}$	0.071
ethylene	$8.52 \times 10^{-12}$	10.013
formaldehyde	$9.37 \times 10^{-12}$	9.330
isobutane	$2.44 \times 10^{-12}$	0.030
isopentane	$3.60 \times 10^{-12}$	0.344
isopropylcyclohexane	$1.34 \times 10^{-11}$	0.126
isopropyltoluene	$8.54 \times 10^{-12}$	0.308
<i>m</i> & <i>p</i> -xylene	$2.31 \times 10^{-11}$	0.319
2-butanone	$1.22 \times 10^{-12}$	1.643
methylbutadiene	$1.05 \times 10^{-10}$	0.091
methylcyclohexane	$5.09 \times 10^{-12}$	0.086
methylcyclopentane	$5.66 \times 10^{-12}$	0.030
<i>n</i> -butane	$2.36 \times 10^{-12}$	0.081
<i>n</i> -butylcyclopentane	$1.01 \times 10^{-11}$	0.137
<i>n</i> -decane	$1.11 \times 10^{-11}$	1.461
<i>n</i> -dodecane	$1.39 \times 10^{-11}$	1.193
<i>n</i> -heptane	$6.76 \times 10^{-12}$	0.040
<i>n</i> -hexane	$5.20 \times 10^{-12}$	0.152
<i>n</i> -nonane	$9.70 \times 10^{-12}$	0.738
<i>n</i> -octane	$8.11 \times 10^{-12}$	0.415
<i>n</i> -pentane	$3.80 \times 10^{-12}$	0.076
<i>n</i> -pentylbenzene	$1.01 \times 10^{-11}$	0.182
<i>n</i> -propylbenzene	$5.80 \times 10^{-12}$	0.137
<i>n</i> -tridecane	$1.53 \times 10^{-11}$	0.526
<i>n</i> -undecane	$1.23 \times 10^{-11}$	1.664
<i>o</i> -xylene	$1.36 \times 10^{-11}$	0.339
<i>n</i> -propane	$1.09 \times 10^{-12}$	0.025
propionaldehyde	$2.20 \times 10^{-11}$	0.541
propylcyclopentane	$1.20 \times 10^{-11}$	0.051
propylene	$2.64 \times 10^{-11}$	2.195
toluene	$5.63 \times 10^{-12}$	1.406
trans-1,2-dimethylcyclopentane	$6.80 \times 10^{-12}$	1.310
trans-1,4-dimethylcyclohexane	$1.19 \times 10^{-11}$	0.056
trans-2-butene	$6.40 \times 10^{-11}$	0.076
trans-2-heptene	$6.80 \times 10^{-11}$	0.030
trans-2-octene	$6.94 \times 10^{-11}$	0.071
trans-2-pentene	$6.70 \times 10^{-11}$	0.046
trans-3-nonene	$7.04 \times 10^{-11}$	0.000
C <sub>12</sub> branched alkane	$1.82 \times 10^{-11}$	1.623
C <sub>13</sub> branched alkane	$1.68 \times 10^{-11}$	1.052
C <sub>14</sub> branched alkane	$1.39 \times 10^{-11}$	0.939
C <sub>15</sub> branched alkane	$1.82 \times 10^{-11}$	0.988
C <sub>16</sub> branched alkane	$1.96 \times 10^{-11}$	0.440
C <sub>17</sub> branched alkane	$2.1 \times 10^{-11}$	0.573
C <sub>18</sub> branched alkane	$2.24 \times 10^{-11}$	0.343
C <sub>19</sub> branched alkane	$2.38 \times 10^{-11}$	0.194
C <sub>20</sub> branched alkane	$2.52 \times 10^{-11}$	0.128
C <sub>21</sub> branched alkane	$2.67 \times 10^{-11}$	0.121
C <sub>22</sub> branched alkane	$2.81 \times 10^{-11}$	8.690
C <sub>12</sub> cyclic alkane	$1.82 \times 10^{-11}$	8.858
C <sub>13</sub> cyclic alkane	$1.68 \times 10^{-11}$	6.299

C <sub>14</sub> cyclic alkane	1.39×10 <sup>-11</sup>	5.723
C <sub>15</sub> cyclic alkane	1.82×10 <sup>-11</sup>	4.372
C <sub>16</sub> cyclic alkane	1.96×10 <sup>-11</sup>	3.711
C <sub>17</sub> cyclic alkane	2.1×10 <sup>-11</sup>	3.382
C <sub>18</sub> cyclic alkane	2.24×10 <sup>-11</sup>	2.115
C <sub>19</sub> cyclic alkane	2.38×10 <sup>-11</sup>	1.181
C <sub>20</sub> cyclic alkane	2.52×10 <sup>-11</sup>	0.748
C <sub>21</sub> cyclic alkane	2.67×10 <sup>-11</sup>	0.629
C <sub>22</sub> cyclic alkane	2.81×10 <sup>-11</sup>	1.167
<i>n</i> -dodecane	1.82×10 <sup>-11</sup>	1.094
<i>n</i> -tridecane	1.68×10 <sup>-11</sup>	0.730
<i>n</i> -tetradecane	1.39×10 <sup>-11</sup>	0.613
<i>n</i> -pentadecane	1.82×10 <sup>-11</sup>	0.456
<i>n</i> -hexadecane	1.96×10 <sup>-11</sup>	0.331
<i>n</i> -heptadecane	2.1×10 <sup>-11</sup>	0.296
<i>n</i> -octadecane	2.24×10 <sup>-11</sup>	0.145
<i>n</i> -nonadecane	2.38×10 <sup>-11</sup>	0.073
<i>n</i> -eicosane	2.52×10 <sup>-11</sup>	0.044
<i>n</i> -heneicosane	2.67×10 <sup>-11</sup>	0.029
<i>n</i> -docosane	2.81×10 <sup>-11</sup>	0.287
pristane	2.44×10 <sup>-11</sup>	0.160
phytane	2.61×10 <sup>-11</sup>	0.208
naphthalene	2.3×10 <sup>-11</sup>	0.023
Phenanthrene	1.3×10 <sup>-11</sup>	0.023

Table S4: VBS and SOM model performance for OA mass at 0%, 13.76%, and 60% IVOC mass fractions

Aftertreatment	Model	Fractional Bias			Fractional Error			R <sup>2</sup>		
		0%	13.6%	60%	0%	13.6%	60%	0%	13.6%	60%
None	VBS	-128%	-13%	77%	136%	84%	91%	0.83	0.92	0.9
	SOM	-125%	-63%	70%	138%	108%	90%	0.83	0.94	0.92
DPF+DOC	VBS	-148%	-121%	-46%	161%	133%	99%	0.77	0.96	0.99
	SOM	-145%	-82%	28%	169%	128%	65%	0.52	0.95	0.99
All	VBS	-134%	-49%	36%	144%	100%	82%	0.81	0.92	0.92
	SOM	-135%	-70%	56%	149%	115%	93%	0.77	0.93	0.93

Table S5: SOM performance for O:C predictions at 0%, 13.76%, and 60% IVOC mass fractions.

Aftertreatment	Fractional Bias			Fractional Error			R <sup>2</sup>		
	0%	13.6%	60%	0%	13.6%	60%	0%	13.6%	60%
None	-18%	-46%	-63%	26%	46%	65%	0.86	0.85	0.69
DPF+DOC	29%	-31%	-84%	35%	36%	84%	0.38	0.02	0.29
All	-3%	-41%	-55%	29%	43%	57%	0.80	0.75	0.49



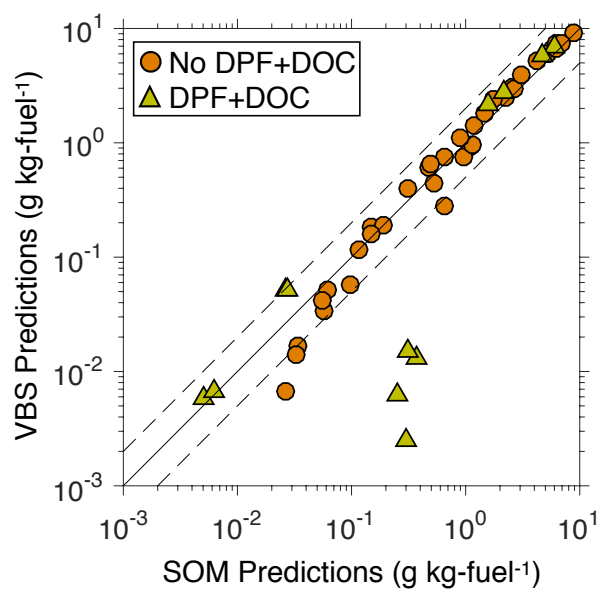


Figure S1: Scatter plot comparing SOM predictions of OA mass to VBS predictions from all experiments at all photochemical ages for the base case.

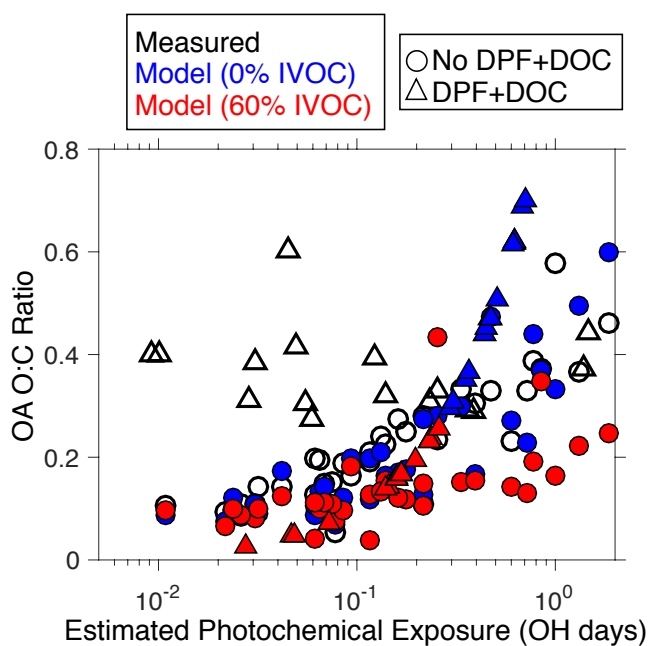


Figure S2: Measurements and model predictions from the 0% and 60% IVOC case of the OA O:C ratio presented as a function of the photochemical age.