Supplement of

Secondary organic aerosol formation from smoldering and flaming combustion of biomass: a box model parametrization based on volatility basis set

Giulia Stefenelli et al.

Correspondence to: Imad El Haddad (imad.el-haddad@psi.ch), Jay G. Slowik (jay.slowik@psi.ch), and Jianhui Jiang (jianhui.jiang@psi.ch)

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Figure S1. Integrated dilution over time calculated for each experiment in Set1 and average dilution ratio across all (Set1) experiments. The average OH exposure at the end of the experiment is $6.3 \times 10^6$ molec cm$^{-3}$ h.
Figure S2. Relative contributions of different primary OGs families (measured in µg m$^{-3}$) for each experiment. The experiments from Set2 (8-14) are ordered based on similarity with Set1 (1-7).
Figure S3. Fraction of consumed precursor compounds for Set2 by OH oxidation (a) and dilution (b) at the end of the experiments. Each point corresponds to a single compound averaged among experiments, accounting for its standard deviation, normalized for initial concentration. The color legend represents the statistical significant deviation from zero reactivity with the investigated reactant ($p$ value).
Figure S4. Reaction rates towards NO$_3$ from NIST database (NIST Chemistry WebBook, 2018) versus amount reacted with the remaining oxidant for different compounds. All data is from Set1 experiments.
Figure S5. Volatility distributions of different precursor classes for Bertrand et al. (2017) (Set1) and Bruns et al. (2016) (Set2), and both of them (labelled "all"). The error bars represent the standard error of 30 bootstrap runs.
Figure S6. Mass yields for each class of compounds for Set1 (a) and Set2 (b). The solid lines represent the median values while the lower and upper limits are the 25th and 75th percentiles, respectively. The shaded background represents the experimental range (20-600 µg m$^{-3}$), outside this shaded area yields are extrapolated from the model.
Figure S7. Mean bias of O:C ratio versus assumed Δ#C.
Table S1. OGs accounted as SOA precursor grouped in different chemical classes. Reported reaction rate constants (cm³ molec⁻¹ s⁻¹) towards OH calculated from Set2 and towards NO₃ from NIST Database. Missing data are not available. Where there is ambiguity regarding the compound identity, the compound listed first is the one for which the NO₃ rate constant is reported. The m/z column denotes the m/z at which the species is actually observed in the PTR-TOF-MS (i.e., protonated mass) and the formula denotes the parent compound.

| m/z | Formula | Identified compound | kOH | kNO₃ |
|-----|---------|---------------------|-----|------|
| **Furans** | | | | |
| 69.03 | C4H4O | Furan | 1.35×10⁻¹ⁱ | 1.4×10⁻¹² |
| 83.05 | C5H6O | 2-Methylfuran | 1.90×10⁻¹ⁱ | 1.1×10⁻¹¹ |
| 85.03 | C4H4O2 | 2-Furanone | 4.91×10⁻¹² | 1.8×10⁻¹³ |
| 97.03 | C5H4O2 | Furan-2-carbaldehyde (furfural) | 1.25×10⁻¹¹ | 2.6×10⁻¹² |
| 97.06 | C6H8O | 2,3/2,4/2.5-dimethylfuran | 2.64×10⁻¹¹ | 5.8×10⁻¹¹/ 5.7×10⁻¹¹/ 5.8×10⁻¹¹ |
| 99.04 | C5H6O2 | 2-methyl-2-butenedial/ Furfuryl alcohol | 9.87×10⁻¹² | |
| 99.08 | C6H10O | Dimethylhydrofurane (Cyclohexanone) | 9.53×10⁻¹³ | |
| 111.08 | C7H10O | Trimethylfuran | 2.47×10⁻¹¹ | |
| 115.04 | C5H6O3 | 4-Methoxy-2(5H)-furanone | 6.89×10⁻¹³ | |
| 117.03 | C8H4O | 2,5-Diethylfuran | | |
| 119.05 | C8H6O | Benzofuran | | |
| 127.04 | C6H6O3 | 5-(hydroxymethyl)furan-2-carbaldehyde/ Hydroxymethylfurfural | 3.19×10⁻¹³ | |
| 141.05 | C7H8O3 | 5-(Methoxymethyl)-2-furaldehyde | | |
| 143.07 | C7H10O3 | 2-Methyl-4,5-dihydro-furan-3-carboxylic acid methyl ester | | |
| **SAH** | | | | |
| 78.05 | C6H5 | Benzene fragment | 4.45×10⁻¹³ | |
| 79.05 | C6H6 | Benzene | 1.37×10⁻¹² | 1.4×10⁻¹⁷ |
| 93.07 | C7H8 | Toluene | 4.85×10⁻¹² | 6.8×10⁻¹⁷ |
| 103.05 | C8H6 | Phenylacetylene | 2.33×10⁻¹¹ | |
| 105.07 | C8H8 | Styrene | 4.12×10⁻¹¹ | |
| 107.09 | C8H10 | Ethylbenzene/1,2-/1,3-/1,4-Xylene | 1.25×10⁻¹¹ | 5.7×10⁻⁹/ 2.0×10⁻⁹/ 7.1×10⁻⁹/ 1.5×10⁻¹⁰ |
| **PAH** | | | | |
| 117.07 | C9H8 | 1-indene | 5.60×10⁻¹¹ | |
| 119.09 | C9H10 | 2-Phenylpropene/2,3-dihydro-1H-indene | 6.59×10⁻¹¹ | 6.8×10⁻¹²/ 6.0×10⁻¹⁵ |
| 129.07 | C10H8 | Naphtalene | 2.14×10⁻¹¹ | |
| 131.09 | C10H10 | Dihydronaphthalene | | |
| 143.09 | C11H10 | Methylnaphtalene | 3.81×10⁻¹¹ | |
| 153.07 | C12H8 | Acenaphytylene | 9.97×10⁻¹¹ | 5.4×10⁻¹² |
| 155.09 | C12H10 | 1,2-dihydro-Acenaphthyrene | 1.09×10⁻¹¹ | 4.6×10⁻¹³ |
| 157.10 | C12H12 | Dimethylnaphtalene | 1.94×10⁻¹¹ | |
| 167.09 | C13H10 | Fluorene | 5.58×10⁻¹¹ | 3.5×10⁻¹⁴ |
| C14H10 | Phenanthrene | 5.45×10^{-12} |
|---|---|---|
| C15H12 | 2-methylantracene | 2.70×10^{-10} |
| C16H10 | Fluoranthenene | 2.99×10^{-12} |
| C6H6O | Phenol | 2.51×10^{-11} |
| C7H6O | Benzaldehyde | 2.0×10^{-15} |
| C6H6O | C6H6O | 2.70×10^{-10} |
| C15H12 | 2-methylanthracene | 2.70×10^{-10} |
| C16H10 | Benzenediol (Catechol)/ methylfurfural | 1.23×10^{-11} |
| C8H8O | 2/3/4-methylbenzaldehyde/ Benzofuran, 2,3-dihydro | 9.8×10^{-13}/ 9.5×10^{-13}/ 9.5×10^{-13}/ 1.1×10^{-13} |
| C7H6O | Hydroxy benzaldehyde | |
| C7H10 | Indenone | |
| C8H10O | Xylenol (2,5-dimethyl phenol) | 7.41×10^{-11} |
| C7H8O2 | Methylbenzenediols/ Guaiacol (2-methoxyphenol) | 2.15×10^{-11} |
| C8H8O2 | 2,4,6-Trimethyl phenol | |
| C7H6O3 | Salicylic acid | |
| C8H10O2 | 1.2/-1.3/-1.4-Dimethoxybenzene | 2.44×10^{-11} |
| C9H10O2 | 2-3-dihydroinden-1-one | 9.10×10^{-12} |
| C10H10O2 | 4-Vinylguaiacol | 6.72×10^{-12} |
| C8H8O3 | 4-hydroxy-3-methoxybenzaldehyde | 4.20×10^{-11} |
| C9H12O2 | 4-ethyl-2-methoxyphenol/1,2-dimethoxy-4- methylbenzene | |
| C8H10O3 | Syringol/2,6-Dimethoxyphenol | 2.07×10^{-11} |
| C10H12O2 | 2-methoxy-4-prop-1-enylphenol | 2.92×10^{-11} |
| C9H10O3 | 1-(4-hydroxy-3-methoxyphenylethanone/2,5- dimethylbenzaldehyde)/3,4-dimethoxybenzaldehyde | 6.70×10^{-12} |
| C10H14O2 | 2-methoxyphenol-4-propylphenol | 2.46×10^{-11} |
| C9H12O3 | 2-6-dimethoxy-4-methylphenol | 3.47×10^{-10} |
| C9H10O4 | 3-4-dimethoxybenzoic acid /4-hydrox-3,5- dimethoxybenzaldehyde/ 4-ethyl-2,6-dimethoxyphenol | 7.74×10^{-12} |
| C10H14O3 | 4-ethyl-2,6-dimethoxyphenol | 2.07×10^{-11} |
| C11H14O3 | 1-3-dimethoxy-2-prop-2-enoxynene | 3.81×10^{-12} |
| C7H8O | Naphthol | 6.08×10^{-11} |
| C7H6O2 | Fluoren-9-one | -1.17×10^{-12} |
| C6H5O | 2-Hydroxyphenololate | 1.66×10^{-11} |
|                  | Molecular Formula | Structure                  | Concentration (ppbv) |
|------------------|-------------------|----------------------------|----------------------|
| 113.10           | C7H12O            | Cyclohexane-1-carboxaldehyde | -3.62×10^{-13}       |
| 115.08           | C6H10O2           |                            | 6.59×10^{-10}        |
| 117.09           | C6H12O2           | Hexanoic acid              | 2.06×10^{-12}        |
| 127.08           | C7H10O2           |                            | 1.73×10^{-11}        |
| 141.09           | C8H12O2           |                            |                     |
| 145.04           | C6H8O4            | Dimethyl fumarate          |                     |
| 147.08           | C10H10O           |                            |                     |
| 57.03            | C3H4O             | Acrolein                   | 7.96×10^{-13}        |
| 71.05            | C4H6O             | Methyl vinyl ketone/Methacrolein/Crotonaldehyde | 1.51×10^{-11} |
| 75.04            | C3H6O2            | Methyl acetate/Propionic acid | 4.41×10^{-13} |
| 81.03            | C5H4O             | Cyclopentadienone          | 6.83×10^{-11}        |
| 85.06            | C5H8O             | 3-methyl-3-buten-2-one     | 1.35×10^{-11}        |
| 87.04            | C4H6O2            | Vinyl acetate              | 2.46×10^{-12}        |
| 87.08            | C5H10O            | Pentanal                   | -2.67×10^{-13}       |
| 89.06            | C4H8O2            | ethyl acetate              | 1.20×10^{-12}        |
| 95.01            | C5H2O2            |                            |                     |
| 96.02            | C5H3O2            |                            |                     |
| 101.06           | C5H8O2            | 2-Butenoic acid, methyl ester, (E)- 2-Propenoic acid, ethyl ester / Methyl methacrylate | 1.61×10^{-12} |
| 103.04           | C4H6O3            |                            |                     |
| 103.04           | C4H6O3            |                            | 8.51×10^{-12}        |
| 103.08           | C5H10O2           | Butanoic acid, methyl ester/ 3-Hydroxy-3-methyl-2-butanoic acid/ n-Propyl acetate/ Propanoic acid, ethyl ester | 1.27×10^{-12} |
| 117.06           | C5H8O3            | Levulinic acid             | 4.53×10^{-12}        |
Table S2. Experimental conditions of published SOA yields for different compounds. Reported the type of reactor deployed and the experimental temperatures investigated (Odum et al., 1996; Takekawa et al., 2003; Johnson et al., 2005; Song et al., 2005; Ng et al., 2007; Henry et al., 2008; Chan et al., 2009; Gómez Alvarez et al., 2009; Shakya and Griffin, 2010; Chan et al., 2010; Nakao et al., 2011; Borrás and Tortajada-Genaro, 2012; Yee et al., 2013; Chen et al., 2016; Li et al., 2016; Ahlberg et al., 2017). Missing data are not specified in the related paper.

| reference          | compound                  | reactor/chamber   | temperature |
|--------------------|---------------------------|-------------------|-------------|
| Ahlberg et al. (2017) | m-xylene                  | flow reactor      |             |
| Song et al. (2005)  | m-xylene                  | smog chamber      | 27°C        |
| Nakao et al. (2011) | m-xylene                  | smog chamber      | 27°C        |
|                    | toluene                    | smog chamber      | 27°C        |
|                    | benzene                    | smog chamber      | 27°C        |
|                    | o-cresol                   | smog chamber      | 27°C        |
|                    | m-cresol                   | smog chamber      | 27°C        |
|                    | phenol                     | smog chamber      | 27°C        |
| Ng et al. (2007)    | m-xylene                  | smog chamber      | 25°C        |
|                    | toluene                    | smog chamber      | 25°C        |
| Li et al. (2016a)   | m-xylene                  | smog chamber      | 27°C        |
|                    | toluene                    | smog chamber      | 27°C        |
|                    | benzene                    | smog chamber      | 27°C        |
|                    | 1,2,4-trimethylbenzene     | smog chamber      | 27°C        |
|                    | 1,2,4,5-trimethylbenzene   | smog chamber      | 27°C        |
| Odum et al. (1996)  | m-xylene                  | outdoor chamber   |             |
|                    | 1,2,4-trimethylbenzene     | outdoor chamber   |             |
| Takekawa et al. (2003)| m-xylene               | smog chamber      | 9°C, 30°C   |
|                    | toluene                    | smog chamber      | 9°C, 30°C   |
|                    | 1,2,4-trimethylbenzene     | smog chamber      | 9°C, 30°C   |
| Borrás et al. (2012)| benzene                   | photoreactor      |             |
|                    | phenol                     | photoreactor      |             |
|                    | catechol                   | photoreactor      |             |
| Johnson et al. (2005)| benzene               | outdoor chamber   | 23°C-32°C   |
|                    | 1,3,5-trimethylbenzene     | outdoor chamber   | 19°C-31°C   |
| Henry et al. (2008) | m-cresol                   | smog chamber      | 20°C-21°C   |
|                    | p-cresol                   | smog chamber      | 20°C-21°C   |
|                    | o-cresol                   | smog chamber      | 20°C-21°C   |
| Yee et al. (2013)   | phenol                     | smog chamber      | 20°C-26°C   |
|                    | guaiacol                   | smog chamber      | 20°C-26°C   |
|                    | syringol                   | smog chamber      | 20°C-26°C   |
| Chan et al. (2009)  | naphtalene                 | smog chamber      | 26°C        |
|                    | 1-methylnaphtalene         | smog chamber      | 26°C        |
|                    | 2-methylnaphtalene         | smog chamber      | 26°C        |
| Chen et al. (2016)  | naphtalene                 | smog chamber      |             |
|                    | 1-methylnaphtalene         | smog chamber      |             |
|                    | 2-methylnaphtalene         | smog chamber      |             |
| Shakya et al. (2010)| naphtalene                 | smog chamber      | 21°C-24°C   |
| Compound                  | Condition          | Temperature  |
|--------------------------|--------------------|--------------|
| methylnaphtalene         | smog chamber       | 21°C-24°C    |
|acenaphthylene            | smog chamber       | 21°C-24°C    |
| biphenyl                 | smog chamber       | 21°C-24°C    |
| Chan et al. (2010)       | methacrolein       | 20°C-21°C    |
|                          | crotonaldehyde     | 20°C-21°C    |
|                          | acrolein           | 20°C-21°C    |
|                          | pentanal           | 20°C-21°C    |
| Gomez Alvarez et al. (2009) | furan             | 25°C         |
|                          | methylfuran        | 25°C         |
| Li et al. (2016b)        | 1,2,3-trimethylbenzene | 27°C     |
|                          | 1,2,5-trimethylbenzene | 27°C     |
Table S3. OH reaction rate constants \( (k_{\text{OH}}) \) (cm\(^3\) molec\(^{-1}\) s\(^{-1}\)) determined for each precursors class from Set2.

| Expt. | Furans  | SAH     | PAH     | OxyAH   | OVOC\(_{<6}\) | OVOC\(_{>6}\) |
|-------|---------|---------|---------|---------|--------------|--------------|
| 1 (−10°C) | 1.34×10\(^{-11}\) | 3.22×10\(^{-12}\) | 2.43×10\(^{-11}\) | 1.99×10\(^{-11}\) | 1.16×10\(^{-11}\) | 7.41×10\(^{-12}\) |
| 2 (−10°C) | 2.19×10\(^{-11}\) | 5.63×10\(^{-12}\) | 5.74×10\(^{-11}\) | 3.85×10\(^{-11}\) | 3.38×10\(^{-11}\) | 2.90×10\(^{-11}\) |
| 3 (+15°C) | 8.41×10\(^{-12}\) | 3.79×10\(^{-12}\) | 3.48×10\(^{-11}\) | 2.37×10\(^{-11}\) | 9.24×10\(^{-12}\) | 5.48×10\(^{-12}\) |
| 4 (+15°C) | 8.91×10\(^{-12}\) | 4.31×10\(^{-12}\) | 3.33×10\(^{-11}\) | 1.87×10\(^{-11}\) | 1.16×10\(^{-11}\) | 5.97×10\(^{-12}\) |
| 5 (+15°C) | 1.36×10\(^{-11}\) | 3.70×10\(^{-12}\) | 1.92×10\(^{-11}\) | 3.09×10\(^{-11}\) | 1.19×10\(^{-11}\) | 7.71×10\(^{-12}\) |
| 6 (+15°C) | 1.22×10\(^{-11}\) | 3.17×10\(^{-12}\) | 2.96×10\(^{-11}\) | 2.73×10\(^{-11}\) | 1.00×10\(^{-11}\) | 7.75×10\(^{-12}\) |
| 7 (+15°C) | 8.52×10\(^{-12}\) | 3.32×10\(^{-12}\) | 3.10×10\(^{-11}\) | 2.09×10\(^{-11}\) | 8.94×10\(^{-12}\) | 7.78×10\(^{-12}\) |
Table S4. Molecular properties of VBS species assuming ΔC = 0.6 due to fragmentation. #C and #H are calculated as averaged values of all chemical species for each precursor category. #O of each precursor class and volatility bins are calculated by the SIMPOL approach (Pankow and Asher, 2008), provided by Eq. (3) in Donahue et al. (2011).
| OA Species | logC* | #C  | #O  | #H  | O:C  | Molecular Weight |
|------------|-------|-----|-----|-----|------|------------------|
| POA        | -1    | 11.00 | 4.11 | 18.24 | 0.374 | 216              |
|            | 0     | 11.75 | 3.43 | 20.12 | 0.292 | 216              |
|            | 1     | 12.50 | 2.73 | 22.32 | 0.218 | 216              |
|            | 2     | 13.25 | 2.01 | 24.84 | 0.152 | 216              |
|            | 3     | 14.00 | 1.27 | 26.68 | 0.091 | 215              |
|            | 4     | 14.75 | 0.51 | 29.84 | 0.035 | 215              |
| Furans     | -1    | 5.53  | 5.15 | 6.13  | 0.932 | 155              |
|            | 0     | 5.53  | 4.68 | 6.13  | 0.847 | 147              |
|            | 1     | 5.53  | 4.21 | 6.13  | 0.761 | 140              |
|            | 2     | 5.53  | 3.73 | 6.13  | 0.675 | 132              |
|            | 3     | 5.53  | 3.25 | 6.13  | 0.588 | 124              |
|            | 4     | 5.53  | 2.76 | 6.13  | 0.500 | 117              |
| SAH        | -1    | 6.77  | 4.95 | 6.77  | 0.731 | 167              |
|            | 0     | 6.77  | 4.47 | 6.77  | 0.660 | 159              |
|            | 1     | 6.77  | 3.99 | 6.77  | 0.589 | 152              |
|            | 2     | 6.77  | 3.50 | 6.77  | 0.517 | 144              |
|            | 3     | 6.77  | 3.00 | 6.77  | 0.444 | 136              |
|            | 4     | 6.77  | 2.50 | 6.77  | 0.370 | 128              |
| PAH        | -1    | 11.52 | 3.99 | 9.50  | 0.347 | 212              |
|            | 0     | 11.52 | 3.48 | 9.50  | 0.302 | 203              |
|            | 1     | 11.52 | 2.96 | 9.50  | 0.257 | 195              |
|            | 2     | 11.52 | 2.44 | 9.50  | 0.212 | 187              |
|            | 3     | 11.52 | 1.91 | 9.50  | 0.166 | 178              |
|            | 4     | 11.52 | 1.36 | 9.50  | 0.118 | 170              |
| OxyAH      | -1    | 8.17  | 4.69 | 8.72  | 0.574 | 182              |
|            | 0     | 8.17  | 4.20 | 8.72  | 0.514 | 174              |
|            | 1     | 8.17  | 3.71 | 8.72  | 0.454 | 166              |
|            | 2     | 8.17  | 3.21 | 8.72  | 0.392 | 158              |
|            | 3     | 8.17  | 2.70 | 8.72  | 0.330 | 150              |
|        |       |     |     |   |     |
|--------|-------|-----|-----|---|-----|
|        |       |  4  |  5  |  6|  7  |
|        |       | OCOC | C   |   |     |
|        |       | C246 | ≥   |   |     |
|        |       |     |  8.17| 2.19| 8.72| 0.268| 142 |
| -1     | 6.42  | 5.01| 8.13 | 0.780 | 165 |
| 0      | 6.42  | 4.53| 8.13 | 0.706 | 158 |
| 1      | 6.42  | 4.05| 8.13 | 0.631 | 150 |
| 2      | 6.42  | 3.57| 8.13 | 0.556 | 142 |
| 3      | 6.42  | 3.08| 8.13 | 0.479 | 134 |
| 4      | 6.42  | 2.58| 8.13 | 0.402 | 126 |
|        |       | OVOC | C66 |   |     |
|        |       |     |  4.00| 5.37| 5.76| 1.342| 140 |
| -1     | 4.00  | 4.91| 5.76 | 1.228 | 132 |
| 0      | 4.00  | 4.45| 5.76 | 1.113 | 125 |
| 1      | 4.00  | 3.99| 5.76 | 0.997 | 118 |
| 2      | 4.00  | 3.52| 5.76 | 0.880 | 110 |
| 3      | 4.00  | 3.05| 5.76 | 0.762 | 103 |
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