# Supplement of
# Modeling studies for SOA formation from $\alpha$-pinene ozonolysis

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## 1 Gas-phase chemistry mechanism for $\alpha$-pinene oxidation

Table S1: Reaction mechanism for the degradation of $\alpha$-pinene according to Chen and Griffin (2005) updated by rate constants from MCM and HOM yields.

| # | Reactants | | Products | Rate constant in $cm^3\,molecule^{-1}\,s^{-1}$ | Ref. |
|---|---|---|---|---|---|
| 1a | APIN + OH | $\rightarrow$ | $RO_2$101 + $RO_2$T | 1.21E-11$\times\exp(444/T)$ | 1, 6 |
| 1b | APIN + OH | $\rightarrow$ | 0.961 $RO_2$101 + 0.961 $RO_2$T + 0.024 HOM$^\dagger$ | 1.21E-11$\times\exp(444/T)$ | 1, 6 |
| 2 | APIN + $NO_3$ | $\rightarrow$ | $RO_2$102 + $RO_2$T | 1.2E-12$\times\exp(490/T)$ | 1, 6 |
| 3a | APIN + $O_3$ | $\rightarrow$ | 0.2 $RO_2$103 + 0.2 CO + 0.8 OH + 0.05 UR101 + 0.15 PINA + 0.15 $H_2O_2$ + 0.33 $RO_2$104 + 0.27 $RO_2$105 + 0.8 $RO_2$T | 8.05E-16$\times\exp(640/T)$ | 1, 6 |
| 3b | APIN + $O_3$ | $\rightarrow$ | 0.1932 $RO_2$103 + 0.1932 CO + 0.7728 OH + 0.0483 UR101 + 0.1449 PINA + 0.1449 $H_2O_2$ + 0.31878 $RO_2$104 + 0.26082 $RO_2$105 + 0.034 HOM$^\dagger$ | 8.05E-16$\times\exp(640/T)$ | 1, 6 |
| 4 | APIN + O3PX | $\rightarrow$ | 0.75 UR103 + 0.25 NOPI | 3.2E-11 | 2 |
| 5 | $RO_2$101 + NO | $\rightarrow$ | 0.2 AP101 + 0.6 PINA + 0.8 $HO_2$ + 0.2 KETH + 0.2 HCHO | 8.8E-13$\times\exp(180.2/T)$ | 2 |
| 6 | $RO_2$101 + $RO_2$T | $\rightarrow$ | 0.7 PINA + $HO_2$ + 0.3 UR107 + $O_2$ | 1.82E-13$\times\exp(416/T)$ | 2 |
| 7 | $RO_2$101 + $HO_2$ | $\rightarrow$ | 0.8 PINA + 0.2 KETH + 0.2 HCHO + OOH1 | 4.1E-13$\times\exp(790/T)$ | 2 |
| 8 | $RO_2$102 + NO | $\rightarrow$ | 0.6 PINA + 1.825 $NO_2$ + 0.175 AP102 + 0.225 KETH + 0.225 HCHO + 0.4 $HO_2$ | 8.8E-13$\times\exp(180.2/T)$ | 2 |
| 9 | $RO_2$102 + $RO_2$T | $\rightarrow$ | 0.795 PINA + 0.795 $NO_2$ + 0.135 AP101 + 0.07 AP102 + $O_2$ | 1.82E-13$\times\exp(416/T)$ | 2 |

| | | | | | |
|---|---|---|---|---|---|
| 10 | $RO_2102 + HO_2$ | $\rightarrow$ | $0.6\,PINA + 0.825\,NO_2 + 0.175\,AP102 + 0.225\,HCHO + 0.225\,HO_2 + 0.175\,OOH1 + 0.825\,OOH2$ | $4.1E\text{-}13 \times \exp(790/T)$ | 2 |
| 11 | $RO_2103 + NO$ | $\rightarrow$ | $0.38\,AP103 + 0.62\,NRPA + 0.62\,HO_2 + 0.62\,NO_2$ | $1.05E\text{-}12 \times \exp(180.2/T)$ | 2, a |
| 12 | $RO_2103 + RO_2T$ | $\rightarrow$ | $NRPA + HO_2 + O_2$ | $1.82E\text{-}13 \times \exp(416/T)$ | 2 |
| 13 | $RO_2103 + HO_2$ | $\rightarrow$ | $NRPA + OOH1$ | $4.1E\text{-}13 \times \exp(790/T)$ | 2 |
| 14 | $RO_2104 + NO$ | $\rightarrow$ | $NO_2 + RO_2108 + RO_28$ | $8.8E\text{-}13 \times \exp(180.2/T)$ | 2 |
| 15 | $RO_2104 + RO_2T$ | $\rightarrow$ | $0.7\,RO_2108 + 0.7\,RO_28 + 0.3\,RP102 + O_2$ | $1.82E\text{-}13 \times \exp(416/T)$ | 2 |
| 16 | $RO_2104 + HO_2$ | $\rightarrow$ | $RO_2108 + RO_28 + OOH2$ | $4.1E\text{-}13 \times \exp(790/T)$ | 2 |
| 17 | $RO_2105 + NO$ | $\rightarrow$ | $HCHO + NO_2 + RO_2109$ | $8.8E\text{-}13 \times \exp(180.2/T)$ | 2 |
| 18 | $RO_2105 + RO_2T$ | $\rightarrow$ | $0.8\,HCHO + 0.8\,RO_2109 + 0.10\,UR105 + 0.05\,RP103 + 0.05\,UR108 + O_2$ | $1.82E\text{-}13 \times \exp(416/T)$ | 2 |
| 19 | $RO_2105 + HO_2$ | $\rightarrow$ | $HCHO + RO_2109 + OOH2$ | $4.1E\text{-}13 \times \exp(790/T)$ | 2 |
| 20 | $PINA + h\nu$ | $\rightarrow$ | $CO + HO_2 + RO_2103$ | Photolysis MCM* | 6, 7 |
| 21 | $PINA + OH$ | $\rightarrow$ | $0.8\,RO_2106 + 0.2\,RO2104 + H_2O$ | 9.1E-11 | 4 |
| 22 | $PINA + NO_3$ | $\rightarrow$ | $RO_2106 + HNO_3$ | 5.4E-14 | 4 |
| 23 | $RO_2106 + NO$ | $\rightarrow$ | $RO_2103 + 0.8\,CO_2 + O_2$ | $1.11\text{-}11 \times \exp(180.2/T)$ | 2 |
| 24 | $RO_2106 + NO_2 + M$ | $\rightarrow$ | $PAN101 + M$ | Refer to reference | 3 |
| 25 | $PAN101$ | $\rightarrow$ | $RO_2106 + NO_2$ | Refer to reference | 3 |
| 26 | $RO_2106 + RO_2T$ | $\rightarrow$ | $0.2\,UR101 + 0.8\,RO_2103 + 0.8\,CO_2 + O_2$ | 5.0E-12 | 2 |
| 27 | $RO_2106 + HO_2$ | $\rightarrow$ | $0.2\,UR101 + O_3$ | $4.3E\text{-}13 \times \exp(1040/T)$ | 2 |
| 28 | $NRPA + h\nu$ | $\rightarrow$ | $CO + HO_2 + RO_2108$ | Photolysis MCM* | 6, 7 |
| 29 | $NRPA + OH$ | $\rightarrow$ | $0.8\,RO_2107 + 0.2\,RO_2104 + H_2O$ | 9.1E-11 | 4 |
| 30 | $NRPA + NO_3$ | $\rightarrow$ | $RO_2107 + HNO_3$ | 5.4E-14 | 4 |
| 31 | $RO_2107 + NO$ | $\rightarrow$ | $NO_2 + CO_2 + RO_2108$ | $1.11\text{-}11 \times \exp(180.2/T)$ | 2 |
| 32 | $RO_2107 + NO_2 + M$ | $\rightarrow$ | $PAN102 + M$ | Refer to reference | 3 |
| 33 | $PAN102$ | $\rightarrow$ | $RO_2107 + NO_2$ | Refer to reference | 3 |
| 34 | $RO_2107 + RO_2T$ | $\rightarrow$ | $0.2\,UR102 + 0.8\,CO_2 + 0.87,RO_2108 + O_2$ | 5.0E-12 | 2 |
| 35 | $RO_2107 + HO_2$ | $\rightarrow$ | $UR102 + O_3$ | $4.3E\text{-}13 \times \exp(1040/T)$ | 2 |
| 36 | $RO_2108 + NO$ | $\rightarrow$ | $0.35\,AP104 + 0.65\,KETH + 0.65\,NO_2 + 0.65\,HO_2$ | $1.24E\text{-}12 \times \exp(180.2/T)$ | 2, a |
| 37 | $RO_2108 + RO_2T$ | $\rightarrow$ | $KETH + HO_2 + O_2$ | $1.82E\text{-}13 \times \exp(416/T)$ | 2 |
| 38 | $RO_2108 + HO_2$ | $\rightarrow$ | $KETH + OOH1$ | $4.1E\text{-}13 \times \exp(790/T)$ | 2 |
| 39 | $RO_2109 + NO$ | $\rightarrow$ | $CO_2 + NO_2 + RO_2108$ | $1.11\text{-}11 \times \exp(180.2/T)$ | 2 |
| 40 | $RO_2109 + NO_2 + M$ | $\rightarrow$ | $PAN103 + M$ | Refer to reference | 3 |
| 41 | $PAN103$ | $\rightarrow$ | $RO_2109 + NO_2$ | Refer to reference | 3 |
| 42 | $RO_2109 + RO_2T$ | $\rightarrow$ | $0.3\,RP101\,0.1\,UR104 + 0.6\,CO_2 + 0.6\,RO_2108 + O_2$ | 5.0E-12 | 2 |

| | | | | | |
|---|---|---|---|---|---|
| 43 | $RO_2$109 + $HO_2$ | → | UR104 + $O_2$ | 4.3E-13$\times \exp(1040/T)$ | 2 |
| 44 | AP101 + OH | → | PINA + $NO_2$ + $H_2O$ | 5.63E-12 | 5 |
| 45 | AP102 + OH | → | $RO_2$108 + $NO_2$ + $H_2O$ | 6.86E-12 | 5 |
| 46 | AP103 + OH | → | NRPA + $NO_2$ + $H_2O$ | 2.53E-12 | 5 |
| 47 | AP104 + OH | → | KETH + $NO_2$ + $H_2O$ | 2.02E-12 | 5 |
| 48 | RP101 + OH | → | UR104 + $O_3$ - $HO_2$ | 2.62E-11 | 5 |
| 49 | RP102 + OH | → | UR106 + $O_3$ - $HO_2$ | 2.36E-11 | 5 |
| 50 | RP103 + OH | → | UR105 + $O_3$ - $HO_2$ | 2.66E-11 | 5 |

† Reactions updated by HOM yields according to Berndt et al. (2016) utilized for cases 5a and 5b of Table 1

a) Yields calculated according to Arey et al. (2001)

References: 1) Atkinson (1997); 2) Jenkin et al. (1997); 3) Griffin et al. (2002); 4) Glasius et al. (1997); 5) Kwok and Atkinson (1995); 6) http://mcm.leeds.ac.uk/MCM/; 7) Saunders et al. (2003)

* Photolysis according to Saunders et al. (2003) with $J = l(\cos(\chi)^m \exp(-n \sec \chi)$ with $\chi$ the solar zenith angle; $l$ = 2.792E-05; $m$ = 0.805; $n$ = 0.338.

Table S2: Abbreviations and full names of the chemical species included in the $\alpha$-pinene oxidation mechanism.

| **Term** | **Description** |
|---|---|
| | **Reactive, fully integrated species** |
| APIN | $\alpha$-pinene |
| PINA | pinonaldehyde |
| NRPA | norpinonaldehyde |
| AP101 | 2-nitrato-3-hydroxy-pinane |
| AP102 | 2-nitrato-3-oxo-pinane |
| AP103 | 2,2-dimethyl-3-acetyl-cyclobutyl-methyl-nitrate |
| AP104 | 2,2-dimethyl-3-acetyl-cyclobutyl-nitrate |
| HOM | highly oxidized organic compound |
| PAN101 | peroxy 2,2-dimethyl-3-acetyl-cyclobutyl-acetyl-nitrate |
| PAN102 | peroxy 2,2-dimethyl-3-acetyl-cyclobutyl-formyl-nitrate |
| PAN103 | peroxy 2,2-dimethyl-3-formylmethyl-cyclobutyl-formyl-nitrate |
| RP101 | pinalic-3-acid |
| RP102 | 1-hydroxy-pinonaldehyde |
| RP103 | 10-hydroxy-pinonaldehyde |
| | **Nonreacting, fully integrated species** |

| | |
|---|---|
| UR101 | pinonic acid |
| UR102 | norpinonic acid |
| UR103 | 2,3-pinane-epoxide |
| UR104 | pinic acid |
| UR105 | 10-hydroxy-pinonic acid |
| UR106 | 1-hydroxy-pinonic acid |
| UR107 | 2,3-dihydroxy-pinane |
| UR108 | 2-(2,2-dimethyl-3-formylmethyl-cyclobutyl)-2-keto-acetaldehyde |
| | **Reactive, organic pseudo-steady species** |
| $RO_2101$ | hydroxy alkyl peroxy radical from oxidation of $\alpha$-pinene (2-peroxy-3-hydroxy-pinane) |
| $RO_2102$ | nitrato alkyl peroxy radical from oxidation of $\alpha$-pinene (65 % is 2-peroxy-3-nitrato-pinane, 35 % is 2-nitrato-3-peroxy-pinane) |
| $RO_2103$ | cyclic keto alkyl peroxy radical from oxidation of $\alpha$-pinene ($C_4$ cycle, 1-methyl peroxy, 2,2-dimethyl, 3-acetyl) |
| $RO_2104$ | cyclic keto aldehydic peroxy radical from oxidation of $\alpha$-pinene ($C_4$ cycle, 1-peroxy, 1-acetyl, 2,2-dimethyl, 3-formylmethyl) |
| $RO_2105$ | cyclic keto alkyl peroxy radical from oxidation of $\alpha$-pinene ($C_4$ cycle, 1-(1-keto-ethyl peroxy), 2,2-dimethyl, 3-formylmethyl) |
| $RO_2106$ | acyl peroxy radical from aldehydic H abstraction of pinonaldehyde |
| $RO_2107$ | acyl peroxy radical from aldehydic H abstraction of norpinonaldehyde |
| $RO_2108$ | cyclic keto alkyl peroxy radical from oxidation of $\alpha$-pinene ($C_4$ cycle, 1-peroxy, 2,2-dimethyl, 3-acetyl) |
| $RO_2109$ | acyl peroxy radical from oxidation of $\alpha$-pinene ($C_4$ cycle, 1-formyl peroxy, 2,2-dimethyl, 3-formylmethyl) |

Table S3: Considered particle phase reactions for $\alpha$-pinene oxidized products required for the kinetic approach and added to the reaction mechanism presented in Table S1.

| # | Reactants | | Products | Rate constant in $s^{-1}$ |
|---|---|---|---|---|
| 51 | pPINA | $\rightarrow$ | rPINA | $1-10^{-6}$ |
| 52 | pRP101 | $\rightarrow$ | rRP101 | $1-10^{-6}$ |
| 53 | pUR104 | $\rightarrow$ | rUR104 | $1-10^{-6}$ |
| 54 | pNRPA | $\rightarrow$ | rNRPA | $1-10^{-6}$ |
| 55 | pRP102 | $\rightarrow$ | rRP102 | $1-10^{-6}$ |
| 56 | pRP103 | $\rightarrow$ | rRP103 | $1-10^{-6}$ |
| 57 | pUR101 | $\rightarrow$ | rUR101 | $1-10^{-6}$ |
| 58 | pUR102 | $\rightarrow$ | rUR102 | $1-10^{-6}$ |
| 59 | pUR105 | $\rightarrow$ | rUR105 | $1-10^{-6}$ |
| 60 | pUR106 | $\rightarrow$ | rUR106 | $1-10^{-6}$ |
| 61 | pAP101 | $\rightarrow$ | rAP101 | $1-10^{-6}$ |
| 62 | pAP102 | $\rightarrow$ | rAP102 | $1-10^{-6}$ |
| 63 | pPAN101 | $\rightarrow$ | rPAN101 | $1-10^{-6}$ |
| 64 | pPAN102 | $\rightarrow$ | rPAN102 | $1-10^{-6}$ |
| 65 | pPAN103 | $\rightarrow$ | rPAN103 | $1-10^{-6}$ |
| 66 | pNOPI | $\rightarrow$ | rNOPI | $1-10^{-6}$ |
| 67 | rPINA | $\rightarrow$ | pPINA | $1-10^{-6}$ |
| 68 | rRP101 | $\rightarrow$ | pRP101 | $1-10^{-6}$ |
| 69 | rUR104 | $\rightarrow$ | pUR104 | $1-10^{-6}$ |
| 70 | rNRPA | $\rightarrow$ | pNRPA | $1-10^{-6}$ |
| 71 | rRP102 | $\rightarrow$ | pRP102 | $1-10^{-6}$ |
| 72 | rRP103 | $\rightarrow$ | pRP103 | $1-10^{-6}$ |
| 73 | rUR101 | $\rightarrow$ | pUR101 | $1-10^{-6}$ |
| 74 | rUR102 | $\rightarrow$ | pUR102 | $1-10^{-6}$ |
| 75 | rUR105 | $\rightarrow$ | pUR105 | $1-10^{-6}$ |
| 76 | rUR106 | $\rightarrow$ | pUR106 | $1-10^{-6}$ |
| 77 | rAP101 | $\rightarrow$ | pAP101 | $1-10^{-6}$ |
| 78 | rAP102 | $\rightarrow$ | pAP102 | $1-10^{-6}$ |
| 79 | rPAN101 | $\rightarrow$ | pPAN101 | $1-10^{-6}$ |

| | | | | |
|---|---|---|---|---|
| 80 | rPAN102 | → | pPAN102 | $1-10^{-6}$ |
| 81 | rPAN103 | → | pPAN103 | $1-10^{-6}$ |
| 82 | rNOPI | → | pNOPI | $1-10^{-6}$ |

Remarks: Reactions 67 – 82 describe the backward reactions considered for the sensitivity studies.

**Table S4.** Estimated vapor pressure of HOMs at 295 K.

| **Substance** | **SIMPOL** | **COSMO-RS*** | **EVAPORATION** |
|---|---|---|---|
| HO-$C_{10}H_{15}(OO)(OOH)_2$ | 8.82E-11 | 9.9E-11 | 5.52E-13 |
| HO-$C_{10}H_{15}(OO)(OOH)ONO_2$ | 1.59E-10 | 8.1E-10 | 7.00E-11 |
| HO-$C_{10}H_{15}(OO)(OOH)OH$ | 1.58E-10 | 2.0E-10 | 6.23E-12 |

* Estimates of COSMO-RS according to Berndt et al. (2016)

## 2 Results

### 2.1 Impact of the particle phase diffusion coefficient $D_b$ on SOA formation

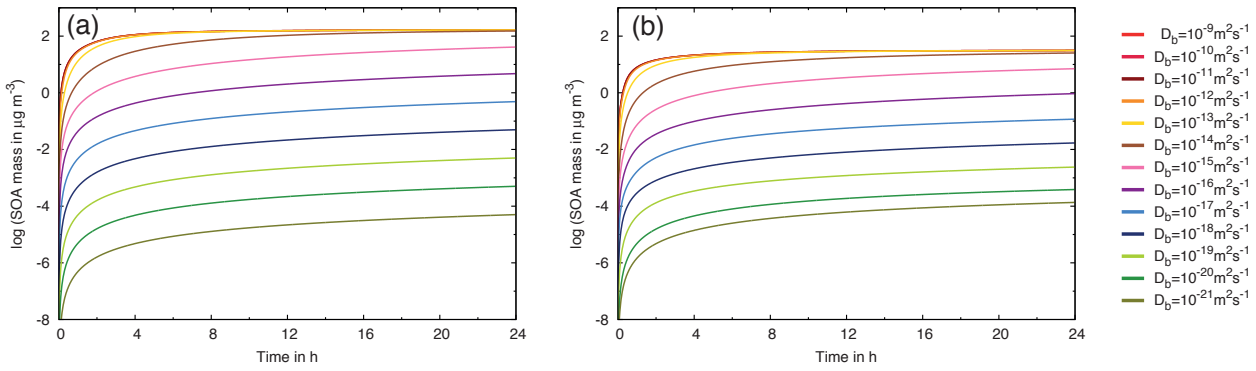


**Figure S1.** Simulated SOA mass for the variation of the bulk particle diffusion coefficient in the range of $D_b$: $10^{-9}$ m$^2$ s$^{-1}$ – $10^{-21}$ m$^2$ s$^{-1}$ (case 1 of Table 1) in logarithmic scale for a) $k_c = 1\,s^{-1}$ and b) $k_c = 10^{-6}\,s^{-1}$.

### 2.2 Impact of the mass accommodation coefficient $\alpha$ on SOA formation

An additional parameter influencing the SOA formation represents the mass accommodation coefficient (see Appendix A), which is defined as the probability to incorporate a molecule penetrating the particle phase boundary in the condensed phase without inducing the direct emission of a molecule of an identical type (Seinfeld and Pandis, 2006). This subsection investigates the sensitivity of SOA formation on the applied mass accommodation coefficient $\alpha$. In the literature different values for the mass accommodation coefficient have been proposed for the uptake of organic compounds in organic particles/ on organic surfaces. Experimental studies show different results than model studies. Saleh et al. (2012) propose an approximate value of $\alpha = 0.4$ from evaporation studies for semi-volatile organic aerosols. In the review of Davidovits et al. (2006) concerning measured mass accommodation coefficients, the uptake values of organic species (e.g. acetic acid, $\alpha$-pinene, $\gamma$-terpinene, p-cymene, and 2-methyl-2-hexanol) on 1-octanol surfaces are summarized. The mass accommodation coefficients are in the range of 0.12 and 0.4 for 265 K, whereby for $\alpha$-pinene only a lower limit with $\alpha > 0.1$ is given. Moreover, Julin et al. (2014) have been combined expansion chamber measurements and molecular dynamics simulations for the determination of the mass accommodation coefficient, where bulk and surface mass accommodation coefficients have been distinguished. The probed organic substances were in liquid, semi-solid or solid phase state. Julin et al. (2014) report surface accommodation coefficients near unity ($0.96 \leq \alpha_s \leq 1$) and the bulk mass accommodation coefficients in the range of $0.14 \leq \alpha_b \leq 1$. Whereby, Julin et al. (2014) state that the conservative lower limits of the bulk mass accommodation coefficients are not very likely, due to the short simulation time scales and near unity values might be consistent with the surface mass accommodation coefficient. Additionally, the lower limit for the bulk mass accommodation coefficient assumes that adsorbed molecules will never enter

the particle bulk, and therefore, only absorbed molecules reach the particle bulk.

According to this wide spread of reported values of the mass accommodation coefficient, we varied $\alpha$ from 1 to $10^{-2}$ for all organic compounds. Further, we investigated these sensitivity studies for different bulk particle phase diffusion coefficients and pseudo-first-order rate constants of particle reactions (see model case 3a and 3b in Table 1). Fig.S2 shows the results of SOA formation for different mass accommodation coefficients and fast particle phase reactions ($k_c = 1$). The SOA mass is highest for $\alpha = 1$. For liquid aerosol particles the simulated SOA mass for $\alpha = 10^{-1}$ in fact leads to about 97 % of the formed SOA mass of the model run using $\alpha = 1$ (see Fig. S2a). For $\alpha = 10^{-2}$ the SOA mass is markedly reduced showing only about 45 % of the maximal simulated value. For nearly semi-solid aerosol particles ($D_b = 10^{-14}$ m$^2$ s$^{-1}$, see Fig. S2b) the SOA formation for $\alpha = 10^{-1}$ is reduced to 15 % of the SOA mass for the simulation with $\alpha = 1$. This demonstrates that the effect on the SOA formation is more substantial when a reduced number of molecules is transferred into the particle surface/bulk and the particle phase diffusion is slower. For semi-solid aerosols ($D_b = 10^{-18}$ m$^2$ s$^{-1}$) the simulation results are similar to those for nearly semi-solid particles with $D_b = 10^{-14}$ m$^2$ s$^{-1}$ and are thus not presented. For moderate particle phase reactions the SOA formation for the reduced mass accommodation coefficients performs in the same way as for fast reactions (see Fig. S2c and S2d).

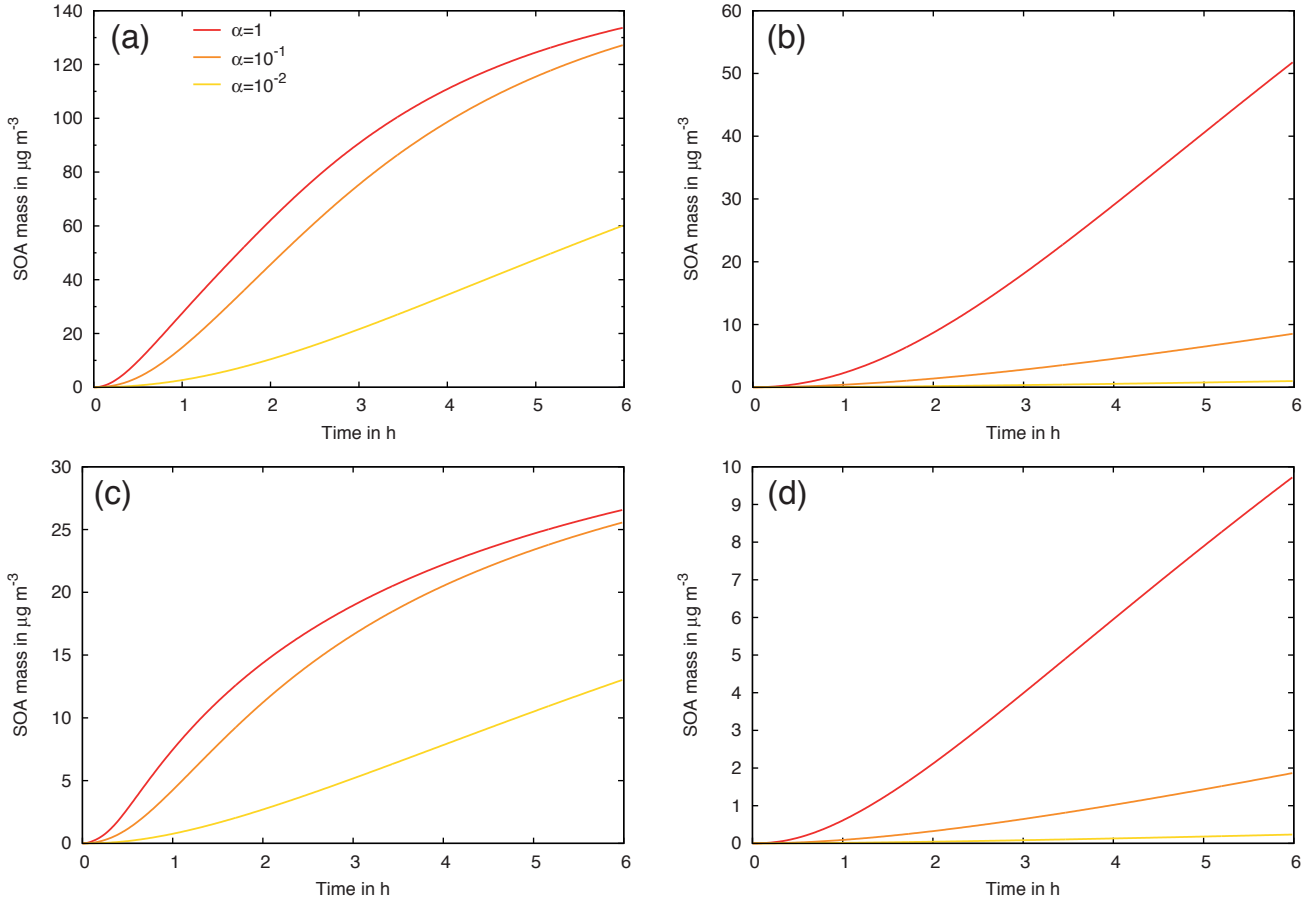


**Figure S2.** Simulated SOA mass for different mass accommodation coefficients for $k_c = 1$ (model case 3a of Table 1) using bulk particle diffusion coefficients for a) liquid ($D_b = 10^{-12}$ m$^2$ s$^{-1}$) and b) the transition between liquid and semi-solid ($D_b = 10^{-14}$ m$^2$ s$^{-1}$) aerosol particles and for $k_c = 10^{-4}$ (model case 3b of Table 1) using bulk particle diffusion coefficients for c) liquid ($D_b = 10^{-12}$ m$^2$ s$^{-1}$) and d) the transition between liquid and semi-solid ($D_b = 10^{-14}$ m$^2$ s$^{-1}$) aerosol particles.

### 2.3 Impact of the initial particle phase organic mass concentration $OM_O$ on SOA formation

Organic material in the aerosol phase serves as an absorptive medium for organic gaseous compounds (see Eq. 4). In order to investigate the dependency of the SOA formation from the initial organic aerosol mass $OM_0$, the initial value has been varied from $10^{-5}$ to $5.8\times10^{-2}$ g g$^{-1}$ (see Table 1, model study 5). Fig. S3 shows the results for the variation of the initial organic mass for liquid and semi-solid particles, whereby $k_c = 10^{-1}$ s$^{-1}$ is held constant. For liquid particles (Fig. S3a) the initial organic mass has a marginal influence on the formed SOA mass because overall high organic mass concentrations occur for this parameter setup. For an intermediate diffusion coefficient $D_b = 10^{-14}$ m$^2$ s$^{-1}$ the effect of the initial organic mass is also insignificant (not shown here). For the semi-solid particles (Fig. S3b) the initial organic mass influences noticeably the formed

SOA mass. However, the total SOA mass is very low and, therefore, the relative influence of the initial organic aerosol mass is increased. The variation of the initial organic particle concentration mass has no significant influence on the formed SOA mass for aerosol particles where effective SOA formation occurs. Additionally, it is noted that a small initial organic particle mass is required for the numerical computation of the equilibrium term, otherwise the partitioning term cannot be calculated (see Eq. 4). This approach is appropriate under ambient conditions.

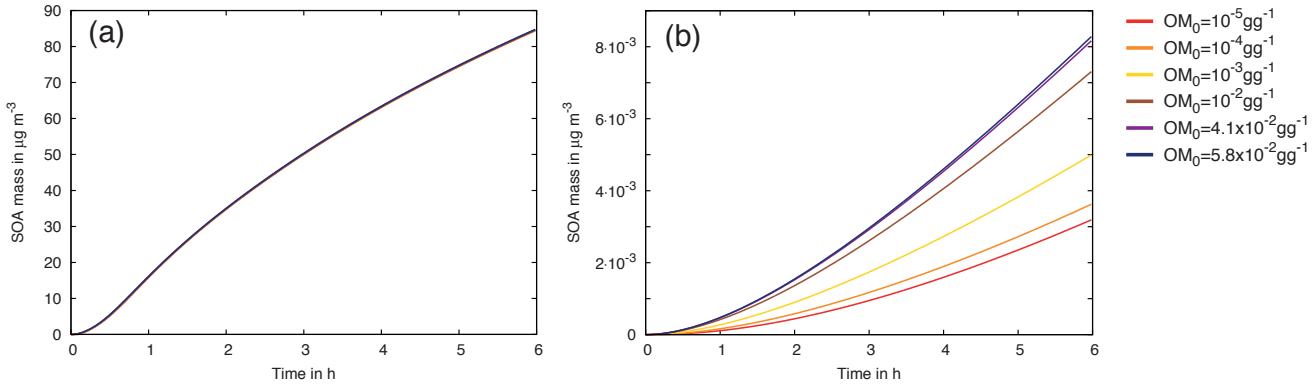


**Figure S3.** Simulated SOA mass formation for different initial particle phase organic mass concentrations $OM_0$ (model case 5 of Table 1) using diffusion coefficients of a) liquid ($D_b = 10^{-12}\,m^2\,s^{-1}$) and b) semi-solid ($D_b = 10^{-18}\,m^2\,s^{-1}$) aerosol particles.

## 2.4 Influence of the particle radius $r_p$ on SOA formation

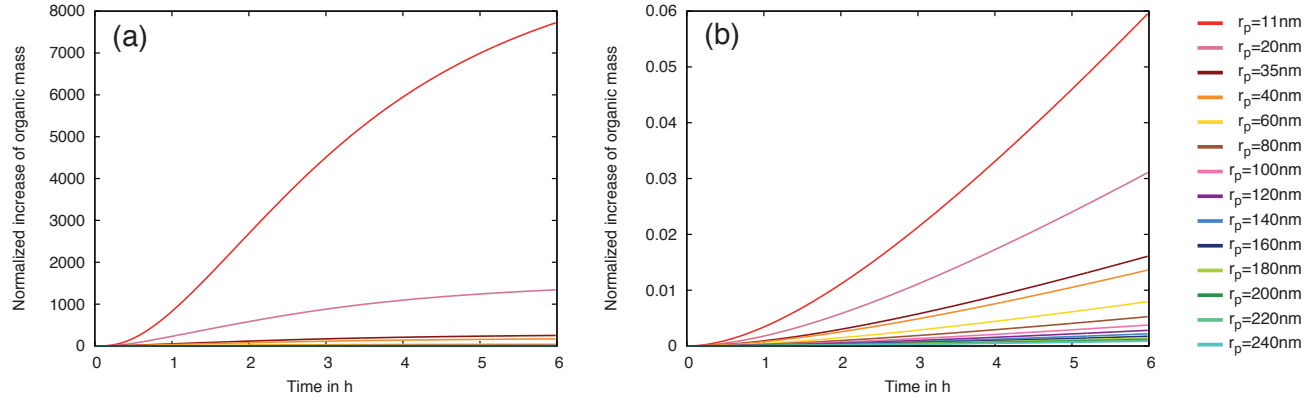


**Figure S4.** Normalized increase of organic mass, which describes the ratio of formed SOA and initial organic mass, for the variation of the particle radius $r_p$ using a constant $k_c = 1\,s^{-1}$ (case 4a and 4b of Table 1); for a) liquid ($D_b = 10^{-12}\,m^2\,s^{-1}$) and b) semi-solid ($D_b = 10^{-18}\,m^2\,s^{-1}$) aerosol particles.

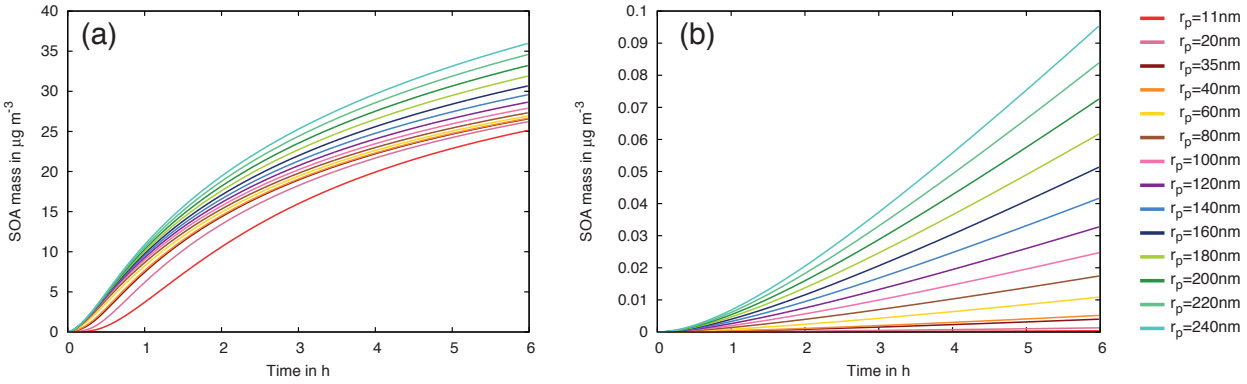


**Figure S5.** Results for the variation of the particle radius $r_\mathrm{p}$ for a constant $k_\mathrm{c} = 10^{-4}\,\mathrm{s}^{-1}$ (case 4b of Table 1) for a) liquid ($D_\mathrm{b} = 10^{-12}\,\mathrm{m}^2\,\mathrm{s}^{-1}$) and b) semi-solid ($D_\mathrm{b} = 10^{-18}\,\mathrm{m}^2\,\mathrm{s}^{-1}$) aerosol particles.

## 2.5 Impact of different HOM vapor pressure estimates on SOA formation

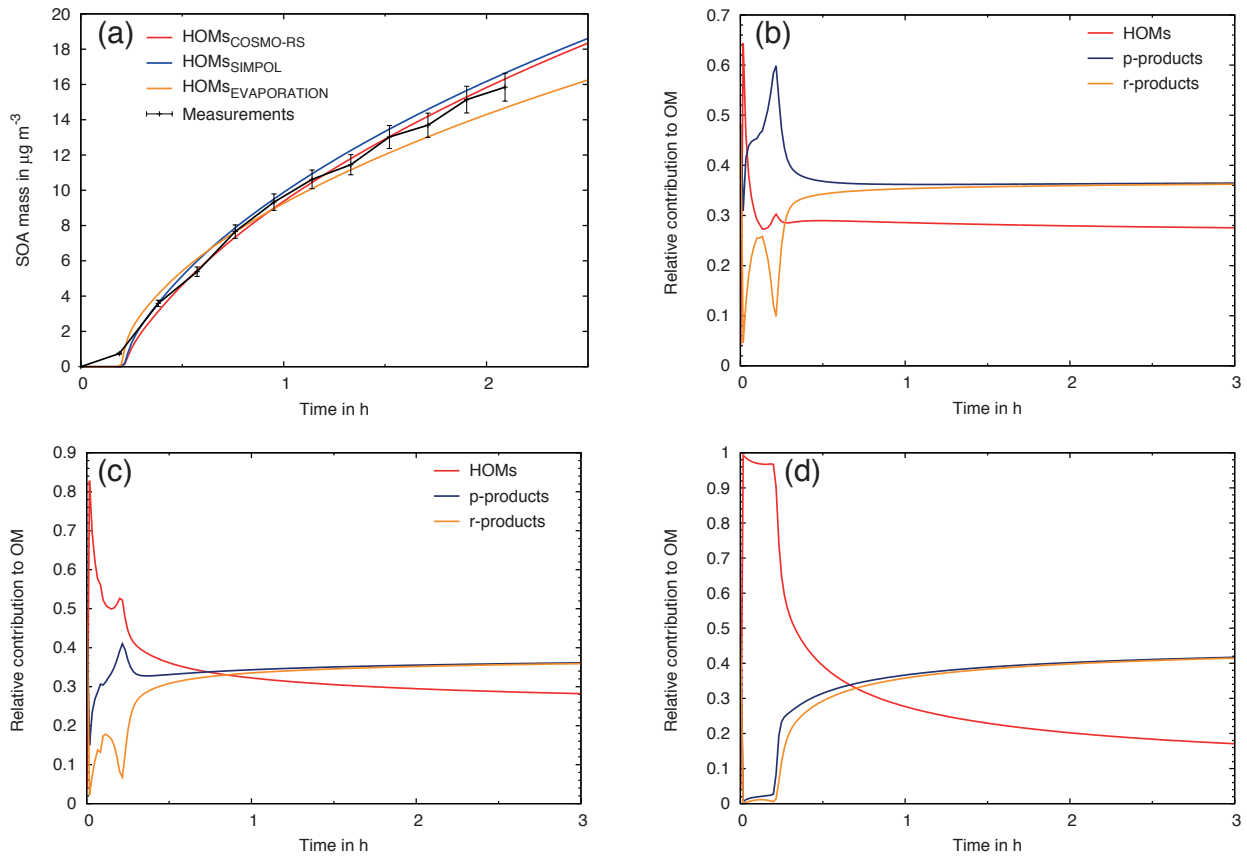


**Figure S6.** Results for the different vapor pressure estimates a) total SOA mass simulated with vapor pressure estimates from COSMO-RS (Eckert and Klamt, 2002), SIMPOL (Pankow and Asher, 2008) and EVAPORATION (Compernolle et al., 2011) and measured SOA mass from the experiment in LEAK. Relative contribution of the individual product classes to the total organic mass for HOM vapor pressures estimated by b) COSMO-RS c) SIMPOL d) EVAPORATION.

## References


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