Supplement of

Influence of atmospheric in-cloud aqueous-phase chemistry on the global simulation of SO₂ in CESM2

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Table S1. Description of all model simulations.

| No. | Case name     | Location in the paper | Chemistry \(^a\) | \([\text{Fe}^{3+}]\) (µM) | pH     |
|-----|---------------|-----------------------|------------------|-----------------|--------|
| 1   | Original      | Sect. 3.1, 3.2, 3.3   | \(a + b\)        |                 |        |
| 2   | Improved      | Sect. 3.2, 3.3, 5.1   | \(a + c + d + e + f + g + h\) | 5  calculated \(^b\) |        |
| 3   | HO\(_x\)-chem | Sect. 4               | \(a + c + d + e\)  |                 |        |
| 4   | Fe-chem       | Sect. 4               | \(a + c + d + f\)  | 5  calculated  |        |
| 5   | N-chem        | Sect. 4               | \(a + c + d + g\)  |                 |        |
| 6   | Carbonate-chem| Sect. 4               | \(a + c + d + h\)  |                 |        |
| 7   | Fe01          | Sect. 5.1             | \(a + c + d + e + f + g + h\) | 0.1 calculated |        |
| 8   | Fe1           | Sect. 5.1             | \(a + c + d + e + f + g + h\) | 1  calculated |        |
| 9   | Fe20          | Sect. 5.1             | \(a + c + d + e + f + g + h\) | 20 calculated |        |
| 10  | Fe100         | Sect. 5.1             | \(a + c + d + e + f + g + h\) | 100 calculated |        |
| 11  | pH3           | Sect. 5.2             | \(a + c + d + e + f + g + h\) | 5  3           |        |
| 12  | pH4           | Sect. 5.2             | \(a + c + d + e + f + g + h\) | 5  4           |        |
| 13  | pH5           | Sect. 5.2             | \(a + c + d + e + f + g + h\) | 5  5           |        |
| 14  | pH6           | Sect. 5.2             | \(a + c + d + e + f + g + h\) | 5  6           |        |
| 15  | HO\(_x\)-pH3 | Sect. 5.2             | \(a + c + d + e\)  |                 | 3      |
| 16  | HO\(_x\)-pH4 | Sect. 5.2             | \(a + c + d + e\)  |                 | 4      |
| 17  | HO\(_x\)-pH5 | Sect. 5.2             | \(a + c + d + e\)  |                 | 5      |
| 18  | HO\(_x\)-pH6 | Sect. 5.2             | \(a + c + d + e\)  |                 | 6      |
| 19  | Fe-pH3        | Sect. 5.2             | \(a + c + d + f\)  | 5  3           |        |
| 20  | Fe-pH4        | Sect. 5.2             | \(a + c + d + f\)  | 5  4           |        |
| 21  | Fe-pH5        | Sect. 5.2             | \(a + c + d + f\)  | 5  5           |        |
| 22  | Fe-pH6        | Sect. 5.2             | \(a + c + d + f\)  | 5  6           |        |
| 23  | N-pH3         | Sect. 5.2             | \(a + c + d + g\)  |                 | 3      |
| 24  | N-pH4         | Sect. 5.2             | \(a + c + d + g\)  |                 | 4      |
| 25  | N-pH5         | Sect. 5.2             | \(a + c + d + g\)  |                 | 5      |
| 26  | N-pH6         | Sect. 5.2             | \(a + c + d + g\)  |                 | 6      |
| 27  | Org-chem      | Sect. 5.3             | \(a + c + d + i\)  |                 |        |

\(^a\) The chemical mechanisms corresponding to different letters are: a. the default MOZART-4 chemistry used in CAM4, b. default parameterized aqueous-phase oxidation reactions of SO\(_2\) used in CAM4, c. gas-aqueous phase transfer equilibria in Table 1a, d. aqueous ionization equilibria, e. HO\(_x\)-chemistry, f. Fe-chemistry, g. N-chemistry, and h. carbonate chemistry in Table 1b, and i. Organic chemistry in Tables S2a and S2b.

\(^b\) The pH values in these simulations are calculated by gas-aqueous phase transfer equilibria in Table 1a and aqueous ionization equilibria in Table 1b.
Table S2a: Gas-aqueous phase transfer equilibria of organic chemistry.

| No. | Reactions | $k_1$ | $k_2$ | Reference |
|-----|-----------|-------|-------|-----------|
| 1$^a$<sup>c</sup> | HCHO(g) → CH$_2$(OH)$_2$<sup>c</sup> | 30 | 0.04 | (Davidovits et al., 2006) |
| 2$^b$ | CH$_2$(OH)$_2$ → HCHO(g) | 3.0 × 10$^3$ | -7.2 × 10$^1$ | (Betterton and Hoffmann, 1988) |
| 3$^a$ | CH$_3$OOH (g) → CH$_3$OOH | 48 | 3.8 × 10$^3$ | (Davidovits et al., 1995) |
| 4$^b$ | CH$_3$OOH → CH$_3$OOH (g) | 6 | -5.32 × 10$^3$ | (Lind and Kok, 1994) |
| 5$^a$ | CH$_3$C(O)OOH (g) → CH$_3$C(O)OOH | 76 | 0.019 | (Herrmann et al., 2000) |
| 6$^b$ | CH$_3$C(O)OOH → CH$_3$C(O)OOH (g) | 6.69 × 10$^2$ | -5.89 × 10$^3$ | (Lind and Kok, 1994) |
| 7$^a$ | CH$_3$OH (g) → CH$_3$OH | 32 | 1.5 × 10$^2$ | (Davidovits et al., 1995) |
| 8$^b$ | CH$_3$OH → CH$_3$OH (g) | 2.2 × 10$^2$ | -5.39 × 10$^3$ | (Betterton, 1992) |
| 9$^a$ | CH$_2$OH(g) → CH$_3$OH | 46 | 8.2 × 10$^3$ | (Davidovits et al., 1995) |
| 10$^b$ | CH$_3$OH → CH$_3$OH (g) | 1.9 × 10$^2$ | -6.29 × 10$^3$ | (Betterton, 1992) |
| 11$^a$ | CH$_3$CHO (g) → CH$_3$CH(OH)$_2$ | 44 | 0.03 | (Herrmann et al., 2000) |
| 12$^b$ | CH$_3$CH(OH)$_2$ → CH$_3$CHO (g) | 11.4 | -6.3 × 10$^3$ | (Betterton and Hoffmann, 1988) |
| 13$^a$ | CH$_3$O$_2$ (g) → CH$_3$O$_2$ | 47 | 3.8 × 10$^3$ | (Herrmann et al., 2000) |
| 14$^b$ | CH$_3$O$_2$ → CH$_3$O$_2$ (g) | 6 | -5.64 × 10$^3$ | (Jacob, 1986) |

$^a$ Reaction rate constant $k = \frac{3 D g LWC}{a r^2}$. The unit is s$^{-1}$. Gas phase diffusion coefficient $D_g = \frac{9.45 \times 10^{17}}{[M]} \sqrt{T(0.03472 + \frac{1}{k_1})}$. LWC is the volume mixing ratio of cloud liquid water. $A = 1 + \left(1 + 1.3 \left(\frac{1}{k_2} - 1\right)\right)$, $\lambda = \frac{0.71 + 1.3\beta}{1 + \beta}$, $\beta = 4.54 \times 10^{-15} \sqrt{V_g^2 + V_{air}^2}$, $V_g = \sqrt{\frac{R T}{\gamma M}}$, $V_{air} = \sqrt{\frac{R T}{28.8 R}}$, $R = 8.31 \times 10^7$ is the ideal gas constant (multiplied by a factor to keep $V_g$ and $V_{air}$ in the unit of cm s$^{-1}$), $r$ is the radius of cloud droplets in cm, [M] is the number density of air in the unit of molecules cm$^{-3}$, $T$ is atmospheric temperature in Kelvin. $k_1$ is the molar mass (g mol$^{-1}$). $k_2$ is the mass accommodation coefficients. All the formulas above refer to (Shao et al., 2019; Liang and Jacobson, 1999).

$^b$ Reaction rate constant $k = \frac{k_{n-1}}{0.082 r LWC C}$. The unit is s$^{-1}$. $C = k_3 \exp \left(-k_2 \left(\frac{1}{7} - \frac{1}{296}\right)\right)$, $k_{n-1}$ is the rate constant of its reverse reaction with $^c$. LWC is as in $^c$. $k_1$ is Henry’s law constants (M atm$^{-1}$) at 298 K. $k_2$ is $\Delta H$ (J mol$^{-1}$) / $R$ (J mol$^{-1}$ K$^{-1}$). $\Delta H$ is the enthalpy of dissolution. All the formulas above refer to (Liang and Jacobson, 1999).

$^c$ All species are liquid species by default, and gas species are marked with (g). The same below.
| No. | Reactions                                                                 | $k_{298}, M^{-1} s^{-1}$ | $E_u/R, K$ | Reference                                      |
|-----|---------------------------------------------------------------------------|--------------------------|------------|-----------------------------------------------|
| 15  | HCHO + H$_2$O $\rightarrow$ CH$_2$(OH)$_2$ | 0.18                     | -4030      | (Bell and Evans, 1966)                        |
| 16  | CH$_3$(OH)$_2$ $\rightarrow$ HCHO + H$_2$O                             | $5.1 \times 10^3$       |            | (Bell and Evans, 1966)                        |
| 17  | CH$_3$CHO + H$_2$O $\rightarrow$ CH$_3$CH(OH)$_2$                      | $1.4 \times 10^4$       | -2500      | (Bell et al., 1956)                           |
| 18  | CH$_3$CH(OH)$_2$ $\rightarrow$ CH$_3$CHO + H$_2$O                   | $5.69 \times 10^3$      |            | (Bell et al., 1956)                           |
| 19  | CH$_3$(OH)$_2$ + HSO$_3^-$ $\rightarrow$ HOCH$_2$SO$_3^-$ + H$_2$O     | 790                      | 2990       | (Olson and Hoffmann, 1989)                     |
| 20  | HOCH$_2$SO$_3^-$ + H$_2$O $\rightarrow$ CH$_2$(OH)$_2$ + HSO$_4^-$     | $3.95 \times 10^{-6}$   | 2990       | (Olson and Hoffmann, 1989)                     |
| 21  | CH$_3$(OH)$_2$ + SO$_2^+$ $\rightarrow$ HOCH$_2$SO$_3^-$ + OH$^-$     | $2.5 \times 10^7$       | 2450       | (Jacobi et al., 1997)                         |
| 22  | HOCH$_2$SO$_3^-$ + OH$^-$ $\rightarrow$ CH$_2$(OH)$_2$ + SO$_2^+$      | $3.7 \times 10^3$       | 4500       | (Deister et al., 1986; Munger et al., 1986)  |
| 23  | NO$_3^-$ + CH$_3$OOH $\rightarrow$ NO$_2^+$ + H$^+$ + CH$_3$O$_2$    | $4.9 \times 10^6$       | 2000       | (Herrmann et al., 2000)                       |
| 24  | HOCH$_2$SO$_3^-$ + OH $\xrightarrow{0.5 H_2O}$ H$_2$O + HO$_2$ + HCOOH + HSO$_3^-$ | $3 \times 10^8$   |            | (Buxton, 1994)                               |
| 25  | HOCH$_2$SO$_3^-$ + SO$_4^-$ $\rightarrow$ SO$_2^+$ + H$^+$ + HCHO + SO$_3^-$ | $2.8 \times 10^6$ |            | (Buxton, 1994)                               |
| 26  | HOCH$_2$SO$_3^-$ + NO$_3^-$ $\rightarrow$ NO$_2^+$ + H$^+$ + HCHO + SO$_3^-$ | $4.2 \times 10^6$ |            | (Herrmann and Zellner, 1998)                 |
| 27  | HSO$_4^-$ + CH$_3$OOH $\xrightarrow{H^+}$ SO$_2^+$ + 2 H$^+$ + CH$_3$OH | $1.8 \times 10^7$       | 3800       | (Lind et al., 1987)                           |
| 28  | HSO$_4^-$ + CH$_3$(C)OOH $\xrightarrow{H^+}$ H$_2$O + HO$_2$ + HCOOH + HSO$_3^-$ | $4.8 \times 10^7$   | 3900       | (Lind et al., 1987)                           |
| 29  | SO$_4^-$ + CH$_3$OOH $\rightarrow$ SO$_2^+$ + H$^+$ + CH$_3$O$_2$      | $2.8 \times 10^7$       |            | (Herrmann et al., 2000)                       |
| 30  | CH$_3$OH + OH $\xrightarrow{0.4}$ H$_2$O + HO$_2$ + HCHO               | $1.0 \times 10^9$       | 580        | (Elliot and Meckraken, 1989)                  |
| 31  | CH$_3$OH + SO$_4^-$ $\xrightarrow{0.4}$ SO$_2^+$ + H$^+$ + HO$_2$ + HCHO | $9.0 \times 10^6$      | 2190       | (Clifton and Huie, 1989)                      |
| 32  | CH$_3$OH + NO$_3^-$ $\xrightarrow{0.4}$ NO$_2^+$ + H$^+$ + HO$_2$ + HCHO | $5.4 \times 10^5$      | 4300       | (Herrmann and Zellner, 1998)                  |
| 33  | CH$_3$OH + CO$_2^-$ $\xrightarrow{0.4}$ CO$_2^+$ + H$^+$ + HO$_2$ + HCHO | $2.6 \times 10^5$      | 4500       | (Chen et al., 1973; Zellner et al., 1996)    |
| 34  | C$_2$H$_5$OH + OH $\xrightarrow{0.4}$ H$_2$O + HO$_2$ + CH$_3$CHO    | $1.9 \times 10^9$       |            | (Buxton et al., 1988)                         |
| 35  | C$_3$H$_6$O + SO$_4^-$ $\xrightarrow{0.4}$ SO$_2^+$ + H$^+$ + HO$_2$ + CH$_3$CHO | $4.1 \times 10^7$   | 1760       | (Clifton and Huie, 1989)                      |
| 36  | C$_3$H$_6$O + NO$_3^-$ $\xrightarrow{0.4}$ NO$_2^+$ + H$^+$ + HO$_2$ + CH$_3$CHO | $2.2 \times 10^6$      | 3300       | (Herrmann and Zellner, 1998)                  |
| 37  | C$_3$H$_6$O + CO$_2^-$ $\xrightarrow{0.4}$ CO$_2^+$ + H$^+$ + HO$_2$ + CH$_3$CHO | $1.5 \times 10^4$      |            | (Kuz'min, 1972)                              |
| 38  | CH$_3$(OH)$_2$ + OH $\xrightarrow{0.4}$ H$_2$O + HO$_2$ + HCOOH       | $1.0 \times 10^9$       | 1020       | (Hart et al., 1964; Chin and Wine, 1994)     |
| 39  | CH$_3$(OH)$_2$ + SO$_4^-$ $\xrightarrow{0.4}$ SO$_2^+$ + H$^+$ + HO$_2$ + HCOOH | $1.4 \times 10^7$      | 1300       | (Buxton et al., 1990)                         |
| 40  | CH$_3$(OH)$_2$ + NO$_3^-$ $\xrightarrow{0.4}$ NO$_2^+$ + H$^+$ + HO$_2$ + HCOOH | $1.0 \times 10^6$      | 4500       | (Exner et al., 1993)                         |
| 41  | CH$_3$(OH)$_2$ + CO$_2^-$ $\xrightarrow{0.4}$ CO$_2^+$ + H$^+$ + HO$_2$ + HCOOH | $1.3 \times 10^4$      |            | (Zellner et al., 1996)                       |
| 42  | CH$_3$CH(OH)$_2$ + OH $\xrightarrow{0.4}$ H$_2$O + HO$_2$ + CH$_3$COOH | $1.2 \times 10^9$      |            | (Schuchmann and Vonsonntag, 1988)            |
| 43  | CH$_3$CHO + OH $\xrightarrow{0.5 H_2O}$ H$_2$O + HO$_2$ + CH$_3$COOH   | $3.6 \times 10^9$       |            | (Schuchmann and Vonsonntag, 1988)            |
| 44  | CH$_3$CH(OH)$_2$ + SO$_4^-$ $\xrightarrow{0.4}$ SO$_2^+$ + H$^+$ + HO$_2$ + CH$_3$COOH | $1 \times 10^7$  |            | (Herrmann et al., 2000)                      |
| 45  | CH$_3$CH(OH)$_2$ + NO$_3^-$ $\xrightarrow{0.4}$ NO$_2^+$ + H$^+$ + HO$_2$ + CH$_3$COOH | $1.9 \times 10^6$      |            | (Zellner et al., 1996)                       |
\[
\begin{align*}
46 & \quad \text{CH}_3\text{CH(OH)}_2 + \text{CO}_3^{2-} \overset{\Delta}{\rightarrow} \text{CO}_2^{3-} + \text{H}^+ + \text{HO}_2 + \text{CH}_3\text{COOH} & 1 \times 10^4 & \text{(Herrmann et al., 2000)} \\
47 & \quad \text{CH}_3\text{COO}^- + \text{SO}_4^{2-} \overset{\Delta}{\rightarrow} \text{SO}_2^{3-} + \text{CH}_3\text{O}_2 + \text{CO}_2 & 2.8 \times 10^7 & 1210 & \text{(Reese et al., 1997; Huie and Clifton, 1999)} \\
48 & \quad \text{CH}_3\text{COO}^- + \text{NO}_3^- \overset{\Delta}{\rightarrow} \text{NO}_5^- + \text{CH}_3\text{O}_2 + \text{CO}_2 & 2.9 \times 10^6 & 3800 & \text{(Exner et al., 1997)} \\
49 & \quad \text{CH}_3\text{COO}^- + \text{CO}_3^{2-} \overset{\Delta}{\rightarrow} \text{CO}_2^{3-} + \text{CH}_3\text{O}_2 + \text{CO}_2 & 580 & \text{(Zellner et al., 1996)} \\
50 & \quad \text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{OH} + \text{HCHO} + \text{O}_2 & 1.7 \times 10^8 & 2200 & \text{(Herrmann et al., 1999)} \\
51 & \quad \text{CH}_3\text{O}_2 + \text{HSO}_4^- \rightarrow \text{CH}_3\text{OH} + \text{SO}_4^{2-} & 5 \times 10^5 & \text{(Herrmann et al., 1999)} \\
52 & \quad \text{CO}_3^{2-} + \text{CH}_3\text{OOH} \rightarrow \text{HCO}_3^- + \text{CH}_3\text{O}_2 & 4.3 \times 10^5 & \text{(Herrmann et al., 2000)} \\
53 & \quad \text{CH}_3\text{O}_2 + \text{O}_2 \overset{\text{H}_2\text{O}}{\rightarrow} \text{CH}_3\text{OOH} + \text{OH}^- + \text{O}_2 & 5.0 \times 10^7 & 1050 & \text{(Jacob, 1986)} \\
54 & \quad \text{CH}_3\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{OH} + \text{OH}^- & 1.9 \times 10^7 & 1850 & \text{(Jacob, 1986)} \\
55 & \quad \text{CH}_3\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{O}_2 + \text{H}_2\text{O} & 2.7 \times 10^7 & 1700 & \text{(Jacob, 1986)} \\
56 & \quad \text{HOCH}_2\text{SO}_3^- + \text{OH} \overset{\Delta}{\rightarrow} \text{CH}_2(\text{OH})_2 + \text{SO}_4^- & 2.6 \times 10^8 & 1500 & \text{(Olson and Fessenden, 1992)} \\
57 & \quad \text{OH} + \text{HOCH}_2\text{SO}_3^- \rightarrow \text{SO}_2^{3-} + \text{H}^+ + \text{HCHO} & 1 \times 10^9 & \text{(Jacob, 1986)} \\
58 & \quad \text{CH}_2(\text{OH})_2 + \text{FeO}^{2+} \overset{\Delta}{\rightarrow} \text{Fe}^{3+} + \text{HCOOH} + \text{HO}_2 + \text{OH}^- & 400 & 5350 & \text{(Jacobsen et al., 1998)} \\
59 & \quad \text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{OOH} + \text{O}_2 & 4.3 \times 10^5 & 3000 & \text{(Jacob, 1986)} \\
60 & \quad \text{HOCH}_2\text{SO}_3^- + \text{OH} \rightarrow \text{CH}_2(\text{OH})_2 + \text{SO}_4^- & 1.4 \times 10^9 & 1500 & \text{(Jacob, 1986)} \\
\end{align*}
\]

\(n = \text{reaction order} - 1\). The units are \(s^{-1}\) for first-order reactions and \(M^{-1} s^{-1}\) for second-order reactions. Reaction rate constant \(k = k_{298} \exp\left(-\frac{E_a}{R \left(\frac{1}{T} - \frac{1}{298}\right)}\right)\).
Figure S1: The relative differences in global seasonally averaged surface SO₂ mixing ratios between the Improved case and the Original case in 2015 after the incorporation of detailed in-cloud aqueous-phase chemical mechanisms (%). DJF, MAM, JJA and SON represent December-January-February, March-April-May, June-July-August and September-October-November, respectively, the same below.

Figure S2: The global seasonal average ratio of net chemical loss rates of surface SO₂ between the Improved case and the Original case in 2015 after the incorporation of detailed in-cloud aqueous-phase chemical mechanisms.
Figure S3: Scatter plots for monthly average SO$_2$ mixing ratios (ppbv) in EU, US, CN and JK in 2015. The black and red points represent the Original and Improved simulations, respectively. Five blue dashed lines indicate 4:1, 2:1, 1:1, 1:2 and 1:4, respectively. “Ori : Obs” and “Imp : Obs” represent the linear regression slopes of “Original case-Observation” and “Improved case-Observation”, respectively. The corresponding monitoring networks are (a) EMEP, (b) EPA, (c) CNEMC and (d) EANET.
Figure S4: Regional monthly-averaged mixing ratios (ppbv) of SO$_2$ in EU, US, CN and JK in 2015. The black, red and green lines represent the Observed, Original-simulated and Improved-simulated mixing ratios, respectively. The blue columns represent the relative differences (%) between Original and Improved simulations. The corresponding monitoring networks are (a) EMEP, (b) EPA, (c) CNEMC and (d) EANET.
Figure S5: The relative differences (%) in global seasonally averaged surface SO$_2$ mixing ratios in 2015 with the incorporation of HO$_x$-chemistry, Fe-chemistry, N-chemistry and carbonate chemistry individually, from top to bottom (case 3-6 – case 1).

Figure S6: The differences in global seasonally averaged surface SO$_2$ mixing ratios (unit: ppbv) in 2015 after changing the soluble [Fe$^{3+}$] concentration levels from 5 μM to 0.1 (top), 1, 20 and 100 μM (bottom) with the detailed aqueous-phase chemical mechanisms (case 7-10 – case 2).
Figure S7: The differences in global seasonally averaged surface SO$_2$ mixing ratios (unit: ppbv) in 2015 at different pH values on the basis of the Improved case with the overall detailed in-cloud aqueous-phase chemical mechanisms (case 11–14 – case 2). The pH values from top to bottom are 3, 4, 5 and 6. [Fe$^{3+}$] is set to 5 μM.

Figure S8: The differences in global seasonally averaged surface SO$_2$ mixing ratios (unit: ppbv) in 2015 at different pH values after the incorporation of N-chemistry individually (case 23–26 – case 5). The pH values from top to bottom are 3, 4, 5 and 6, respectively.
Figure S9: The differences in global seasonally averaged surface SO$_2$ mixing ratios (unit: ppbv) in 2015 at different pH values after the incorporation of HO$_x$-chemistry individually (case 15–18 – case 3). The pH values from top to bottom are 3, 4, 5 and 6, respectively.

[Fe$^{3+}$] is set to 5 μM.

Figure S10: The differences in global seasonally averaged surface SO$_2$ mixing ratios (unit: ppbv) in 2015 at different pH values after the incorporation of Fe-chemistry individually (case 19–22 – case 4). The pH values from top to bottom are 3, 4, 5 and 6, respectively. [Fe$^{3+}$] is set to 5 μM.
Figure S11: The differences in global seasonally averaged surface SO$_2$ mixing ratios (unit: ppbv) in 2015 with the incorporation of organic chemistry (case 27 – case 3).
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