



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	[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		calculated
4	Fe-chem	Sect. 4	a + c + d + f	5	calculated
5	N-chem	Sect. 4	a + c + d + g		calculated
6	Carbonate-chem	Sect. 4	a + c + d + h		calculated
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		calculated

^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 SO₂ 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
Gas-aqueous phase transfer				
1 ^{a, c}	HCHO(g) → CH ₂ (OH) ₂ ^c	30	0.04	(Davidovits et al., 2006)
2 ^b	CH ₂ (OH) ₂ → HCHO(g)	3.0 × 10 ³	-7.2 × 10 ³	(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	C ₂ H ₅ OH (g) → C ₂ H ₅ OH	46	8.2 × 10 ⁻³	(Davidovits et al., 1995)
10 ^b	C ₂ H ₅ OH → C ₂ H ₅ 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. $A = 1 + \left(\lambda + 1.3 \left(\frac{1}{k_2} - 1 \right) \right)$, $\lambda = \frac{0.71 + 1.3\beta}{1+\beta}$, $\beta = 4.54 \times 10^{-15} \sqrt{V_g^2 + V_{air}^2}$, $V_g = \sqrt{\frac{8RT}{\pi k_1}}$, $V_{air} = \sqrt{\frac{8RT}{28.8\pi}}$, $R = 8.31 \times 10^7$ 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. k₁ is the molar mass (g mol⁻¹). k₂ is the mass accommodation coefficients. All the formulas above refer to (Shao et al., 2019; Liang and Jacobson, 1999).

^b Reaction rate constant $k = \frac{k_{n-1}}{0.082 T LWC C}$. The unit is s⁻¹. $C = k_1 \exp \left(-k_2 \left(\frac{1}{T} - \frac{1}{298} \right) \right)$, k_{n-1} is the rate constant of its reverse reaction with ^a. LWC is as in ^a. k₁ is Henry's law constants (M atm⁻¹) at 298 K. k₂ is ΔH (J mol⁻¹) / R (J mol⁻¹ K⁻¹). ΔH 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.

Table S2b. Aqueous-phase chemistry.

No.	Reactions	k_{298} , M ⁻ⁿ s ⁻¹ ^a	E _a /R, K	Reference
Organic Chemistry				
15	HCHO + H ₂ O → CH ₂ (OH) ₂	0.18	-4030	(Bell and Evans, 1966)
16	CH ₂ (OH) ₂ → HCHO + H ₂ O	5.1 × 10 ⁻³		(Bell and Evans, 1966)
17	CH ₃ CHO + H ₂ O → CH ₃ CH(OH) ₂	1.4 × 10 ⁻⁴	-2500	(Bell et al., 1956)
18	CH ₃ CH(OH) ₂ → CH ₃ CHO + H ₂ O	5.69 × 10 ⁻³		(Bell et al., 1956)
19	CH ₂ (OH) ₂ + HSO ₃ ⁻ → HOCH ₂ SO ₃ ⁻ + H ₂ O	790	2990	(Olson and Hoffmann, 1989)
20	HOCH ₂ SO ₃ ⁻ + H ₂ O → CH ₂ (OH) ₂ + HSO ₃ ⁻	3.95 × 10 ⁻⁶	2990	(Olson and Hoffmann, 1989)
21	CH ₂ (OH) ₂ + SO ₃ ²⁻ → HOCH ₂ SO ₃ ⁻ + OH ⁻	2.5 × 10 ⁷	2450	(Jacobi et al., 1997)
22	HOCH ₂ SO ₃ ⁻ + OH ⁻ → CH ₂ (OH) ₂ + SO ₃ ²⁻	3.7 × 10 ³	4500	(Deister et al., 1986; Munger et al., 1986)
23	NO ₃ + CH ₃ OOH → NO ₃ ⁻ + H ⁺ + CH ₃ O ₂	4.9 × 10 ⁶	2000	(Herrmann et al., 2000)
24	HOCH ₂ SO ₃ ⁻ + OH → ^{O₂,H₂O} H ₂ O + HO ₂ + HCOOH + HSO ₃ ⁻	3 × 10 ⁸		(Buxton, 1994)
25	HOCH ₂ SO ₃ ⁻ + SO ₄ ²⁻ → SO ₄ ²⁻ + H ⁺ + HCHO + SO ₃ ⁻	2.8 × 10 ⁶		(Buxton, 1994)
26	HOCH ₂ SO ₃ ⁻ + NO ₃ → NO ₃ ⁻ + H ⁺ + HCHO + SO ₃ ⁻	4.2 × 10 ⁶		(Herrmann and Zellner, 1998)
27	HSO ₃ ⁻ + CH ₃ OOH → ^{H⁺} SO ₄ ²⁻ + 2 H ⁺ + CH ₃ OH	1.8 × 10 ⁷	3800	(Lind et al., 1987)
28	HSO ₃ ⁻ + CH ₃ C(O)OOH → ^{H⁺} SO ₄ ²⁻ + 2 H ⁺ + CH ₃ COOH	4.8 × 10 ⁷	3900	(Lind et al., 1987)
29	SO ₄ ²⁻ + CH ₃ OOH → SO ₄ ²⁻ + H ⁺ + CH ₃ O ₂	2.8 × 10 ⁷		(Herrmann et al., 2000)
30	CH ₃ OH + OH → ^{O₂} H ₂ O + HO ₂ + HCHO	1.0 × 10 ⁹	580	(Elliot and Mccracken, 1989)
31	CH ₃ OH + SO ₄ ²⁻ → ^{O₂} SO ₄ ²⁻ + H ⁺ + HO ₂ + HCHO	9.0 × 10 ⁶	2190	(Clifton and Huie, 1989)
32	CH ₃ OH + NO ₃ → ^{O₂} NO ₃ ⁻ + H ⁺ + HO ₂ + HCHO	5.4 × 10 ⁵	4300	(Herrmann and Zellner, 1998)
33	CH ₃ OH + CO ₃ ²⁻ → ^{O₂} CO ₃ ²⁻ + H ⁺ + HO ₂ + HCHO	2.6 × 10 ³	4500	(Chen et al., 1973; Zellner et al., 1996)
34	C ₂ H ₅ OH + OH → ^{O₂} H ₂ O + HO ₂ + CH ₃ CHO	1.9 × 10 ⁹		(Buxton et al., 1988)
35	C ₂ H ₅ OH + SO ₄ ²⁻ → ^{O₂} SO ₄ ²⁻ + H ⁺ + HO ₂ + CH ₃ CHO	4.1 × 10 ⁷	1760	(Clifton and Huie, 1989)
36	C ₂ H ₅ OH + NO ₃ → ^{O₂} NO ₃ ⁻ + H ⁺ + HO ₂ + CH ₃ CHO	2.2 × 10 ⁶	3300	(Herrmann and Zellner, 1998)
37	C ₂ H ₅ OH + CO ₃ ²⁻ → ^{O₂} CO ₃ ²⁻ + H ⁺ + HO ₂ + CH ₃ CHO	1.5 × 10 ⁴		(Kuz'min, 1972)
38	CH ₂ (OH) ₂ + OH → ^{O₂} H ₂ O + HO ₂ + HCOOH	1.0 × 10 ⁹	1020	(Hart et al., 1964; Chin and Wine, 1994)
39	CH ₂ (OH) ₂ + SO ₄ ²⁻ → ^{O₂} SO ₄ ²⁻ + H ⁺ + HO ₂ + HCOOH	1.4 × 10 ⁷	1300	(Buxton et al., 1990)
40	CH ₂ (OH) ₂ + NO ₃ → ^{O₂} NO ₃ ⁻ + H ⁺ + HO ₂ + HCOOH	1.0 × 10 ⁶	4500	(Exner et al., 1993)
41	CH ₂ (OH) ₂ + CO ₃ ²⁻ → ^{O₂} CO ₃ ²⁻ + H ⁺ + HO ₂ + HCOOH	1.3 × 10 ⁴		(Zellner et al., 1996)
42	CH ₃ CH(OH) ₂ + OH → ^{O₂} H ₂ O + HO ₂ + CH ₃ COOH	1.2 × 10 ⁹		(Schuchmann and Vonsonntag, 1988)
43	CH ₃ CHO + OH → ^{O₂,H₂O} H ₂ O + HO ₂ + CH ₃ COOH	3.6 × 10 ⁹		(Schuchmann and Vonsonntag, 1988)
44	CH ₃ CH(OH) ₂ + SO ₄ ²⁻ → ^{O₂} SO ₄ ²⁻ + H ⁺ + HO ₂ + CH ₃ COOH	1 × 10 ⁷		(Herrmann et al., 2000)
45	CH ₃ CH(OH) ₂ + NO ₃ → ^{O₂} NO ₃ ⁻ + H ⁺ + HO ₂ + CH ₃ COOH	1.9 × 10 ⁶		(Zellner et al., 1996)

46	$\text{CH}_3\text{CH}(\text{OH})_2 + \text{CO}_3^{2-} \xrightarrow{\text{O}_2} \text{CO}_3^{2-} + \text{H}^+ + \text{HO}_2 + \text{CH}_3\text{COOH}$	1×10^4		(Herrmann et al., 2000)
47	$\text{CH}_3\text{COO}^- + \text{SO}_4^{2-} \xrightarrow{\text{O}_2} \text{SO}_4^{2-} + \text{CH}_3\text{O}_2 + \text{CO}_2$	2.8×10^7	1210	(Reese et al., 1997; Huie and Clifton, 1990)
48	$\text{CH}_3\text{COO}^- + \text{NO}_3^- \xrightarrow{\text{O}_2} \text{NO}_3^- + \text{CH}_3\text{O}_2 + \text{CO}_2$	2.9×10^6	3800	(Exner et al., 1994)
49	$\text{CH}_3\text{COO}^- + \text{CO}_3^{2-} \xrightarrow{\text{O}_2} \text{CO}_3^{2-} + \text{CH}_3\text{O}_2 + \text{CO}_2$	580		(Zellner et al., 1996)
50	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{OH} + \text{HCHO} + \text{O}_2$	1.7×10^8	2200	(Herrmann et al., 1999)
51	$\text{CH}_3\text{O}_2 + \text{HSO}_3^- \rightarrow \text{CH}_3\text{OOH} + \text{SO}_3^-$	5×10^5		(Herrmann et al., 1999)
52	$\text{CO}_3^- + \text{CH}_3\text{OOH} \rightarrow \text{HCO}_3^- + \text{CH}_3\text{O}_2$	4.3×10^5		(Herrmann et al., 2000)
53	$\text{CH}_3\text{O}_2 + \text{O}_2^- \xrightarrow{\text{H}_2\text{O}} \text{CH}_3\text{OOH} + \text{OH}^- + \text{O}_2$	5.0×10^7	1050	(Jacob, 1986)
54	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow \text{CH}_2(\text{OH})_2 + \text{OH}$	1.9×10^7	1850	(Jacob, 1986)
55	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{O}_2 + \text{H}_2\text{O}$	2.7×10^7	1700	(Jacob, 1986)
56	$\text{HOCH}_2\text{SO}_3^- + \text{OH} \xrightarrow{\text{O}_2} \text{CH}_2(\text{OH})_2 + \text{SO}_5^-$	2.6×10^8	1500	(Olson and Fessenden, 1992)
57	$\text{OH} + \text{HOCH}_2\text{SO}_3^- \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{HCHO}$	1×10^9		(Jacob, 1986)
58	$\text{CH}_2(\text{OH})_2 + \text{FeO}^{2+} \xrightarrow{\text{O}_2} \text{Fe}^{3+} + \text{HCOOH} + \text{HO}_2 + \text{OH}^-$	400	5350	(Jacobsen et al., 1998)
59	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{OOH} + \text{O}_2$	4.3×10^5	3000	(Jacob, 1986)
60	$\text{HOCH}_2\text{SO}_3^- + \text{OH} \rightarrow \text{CH}_2(\text{OH})_2 + \text{SO}_3^-$	1.4×10^9	1500	(Jacob, 1986)

^a n = 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 = $k_{298}\exp(-\frac{E_a}{R}(\frac{1}{T} - \frac{1}{298}))$.

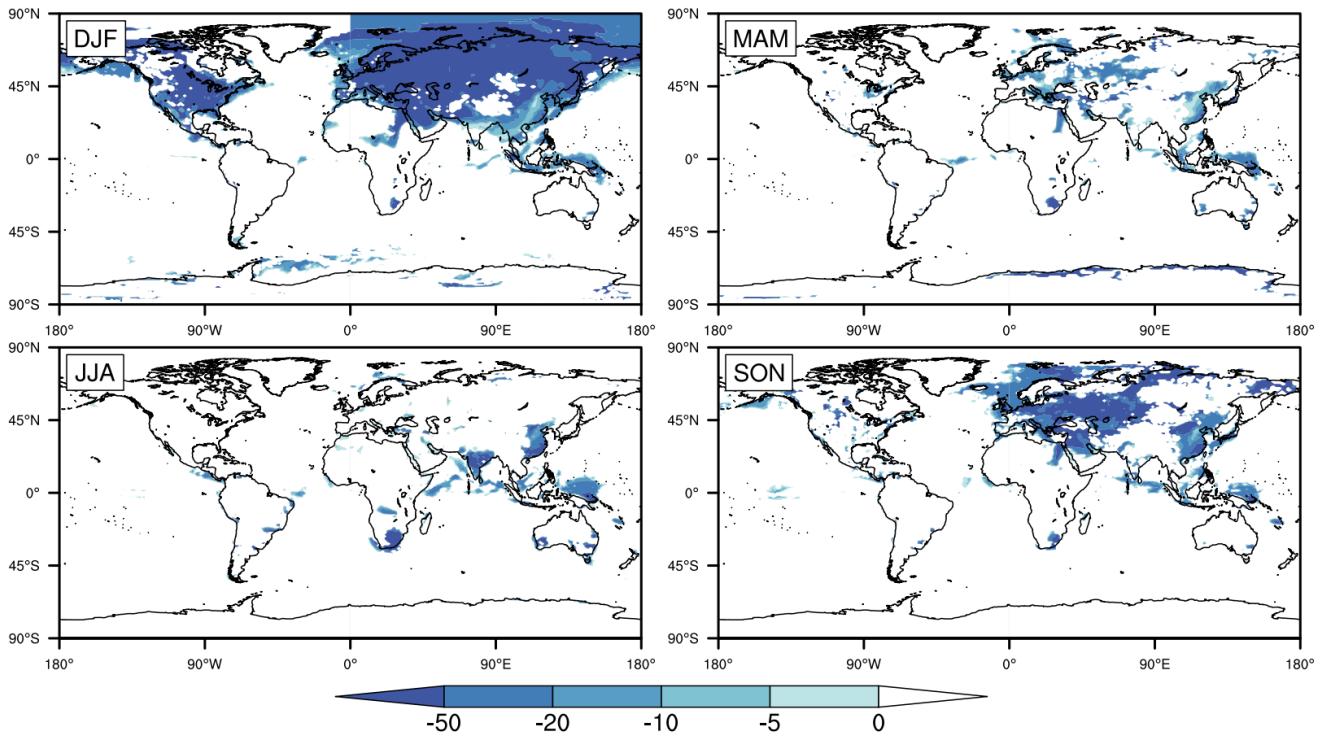


Figure S1: The relative differences in global seasonally averaged surface SO_2 mixing ratios between the Improved case and the Original case in 2015 after the incorporation of detailed in-cloud aqueous-phase chemical mechanisms (%). DJF, MAM, JJA and SON represent December-January-February, March-April-May, June-July-August and September-October-November, respectively, the same below.

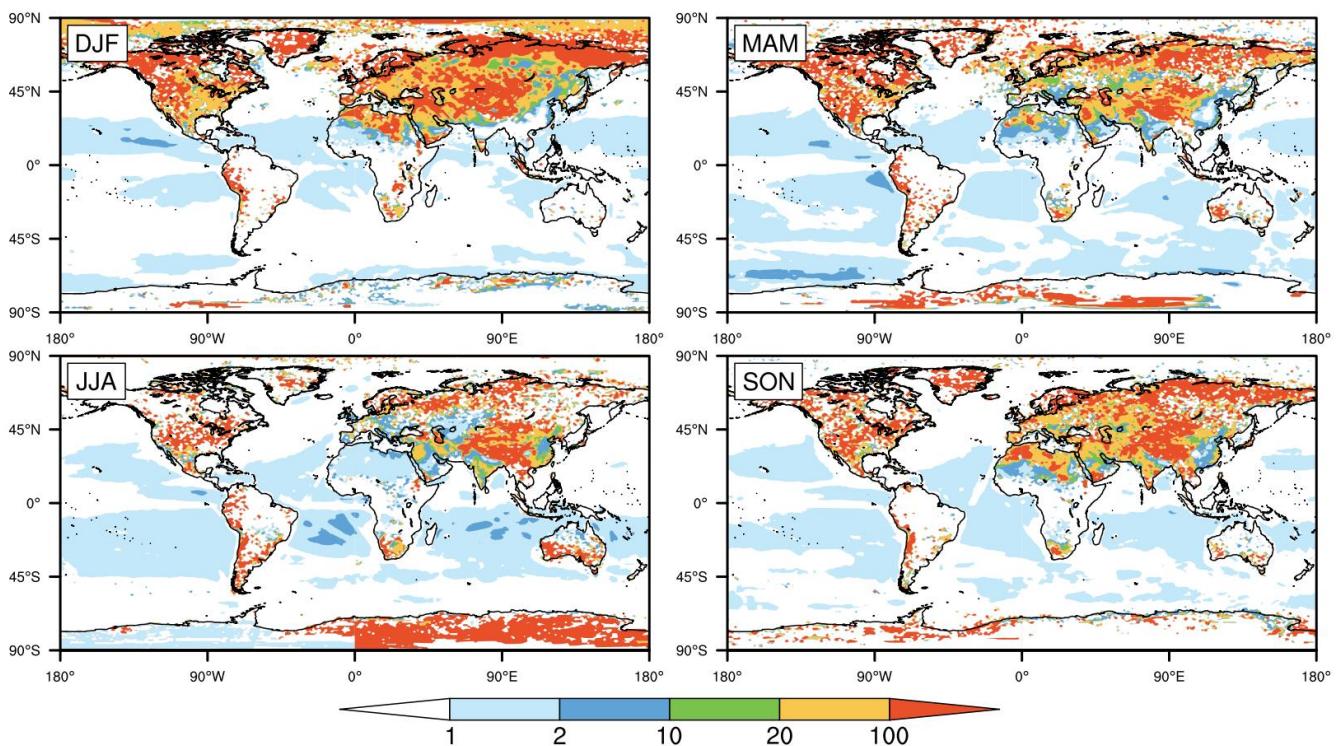


Figure S2: The global seasonal average ratio of net chemical loss rates of surface SO_2 between the Improved case and the Original case in 2015 after the incorporation of detailed in-cloud aqueous-phase chemical mechanisms.

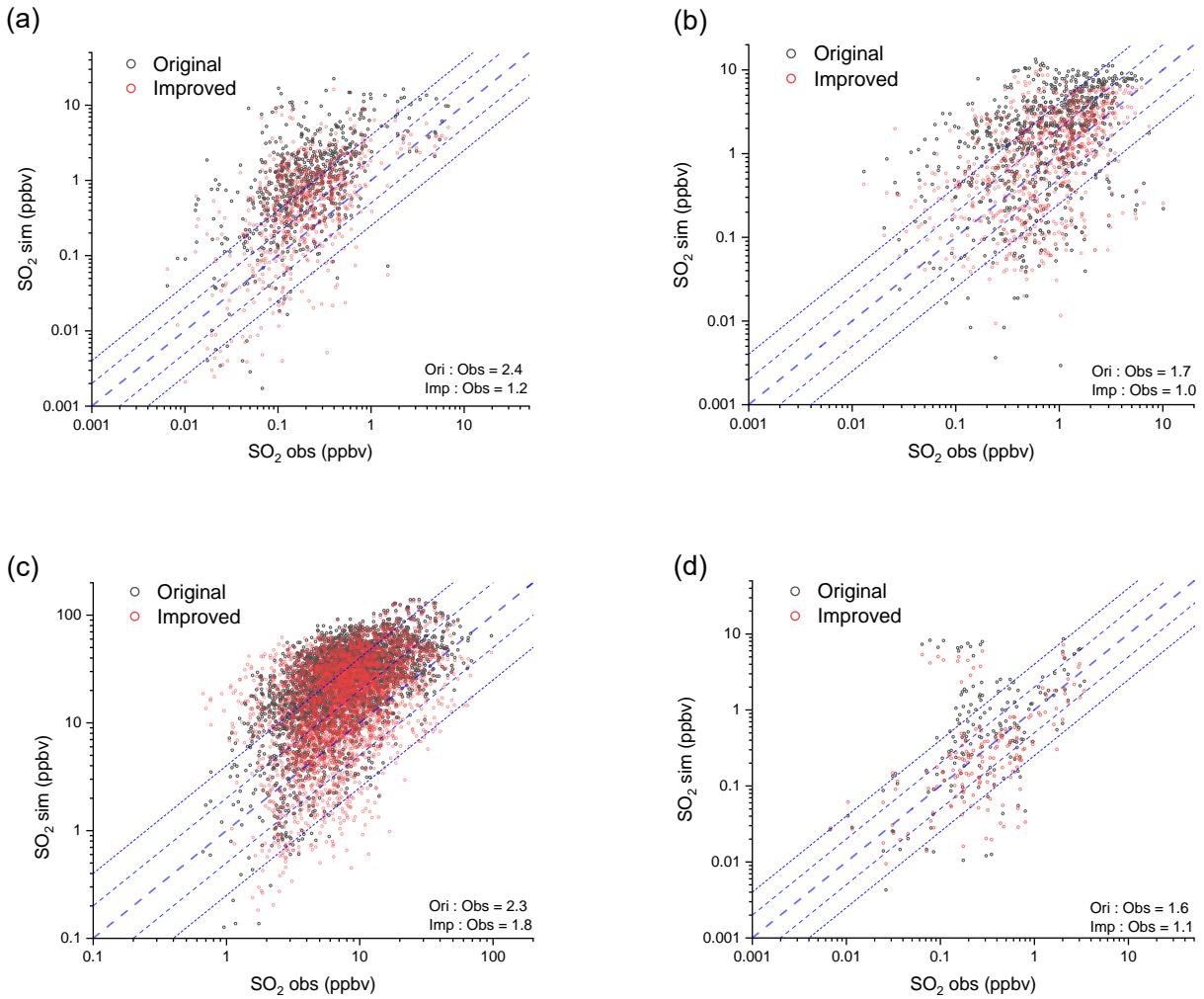


Figure S3: Scatter plots for monthly average SO₂ mixing ratios (ppbv) in EU, US, CN and JK in 2015. The black and red points represent the Original and Improved simulations, respectively. Five blue dashed lines indicate 4:1, 2:1, 1:1, 1:2 and 1:4, respectively. “Ori : Obs” and “Imp : Obs” represent the 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.

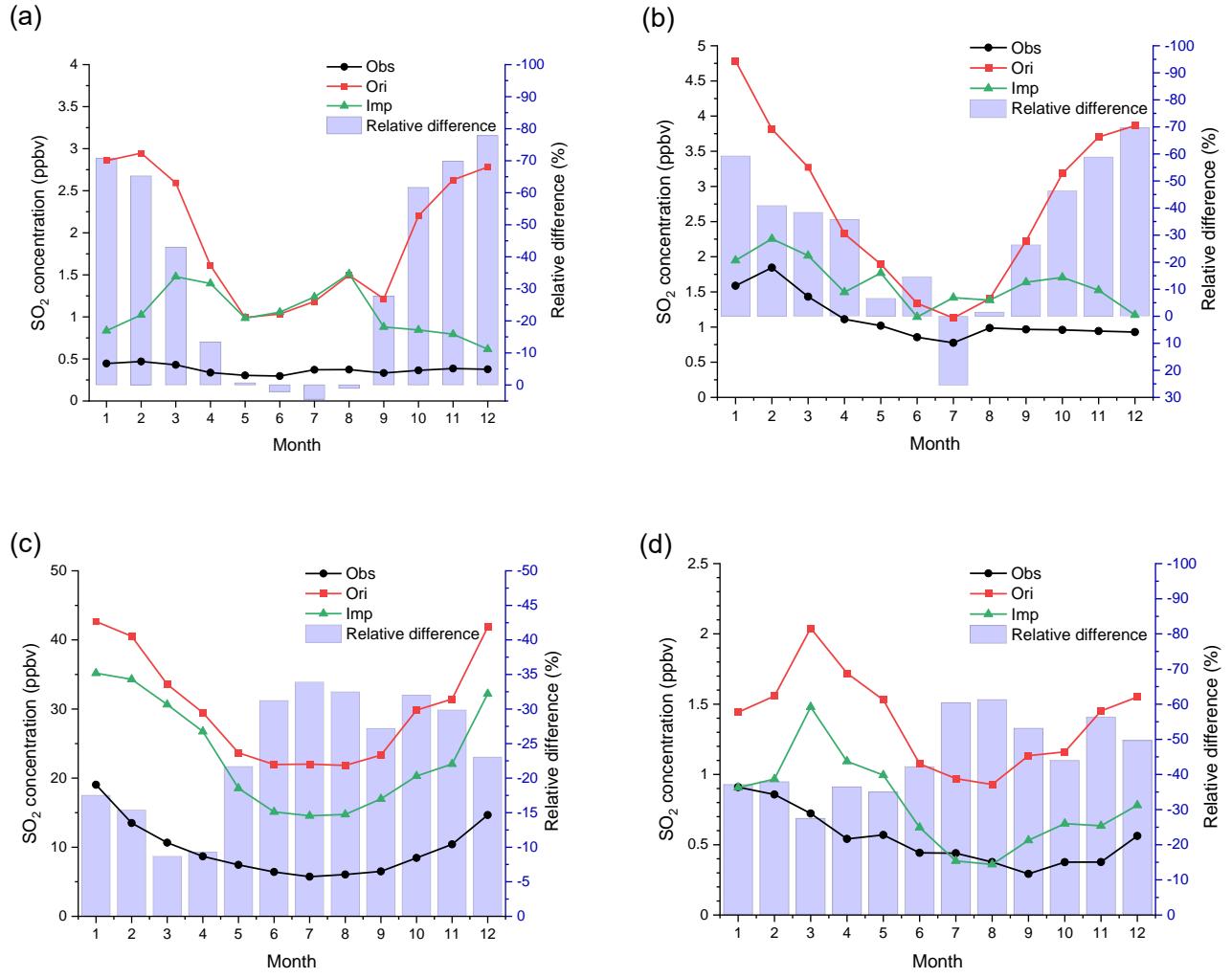


Figure S4: Regional monthly-averaged mixing ratios (ppbv) of SO₂ in EU, US, CN and JK in 2015. The black, red and green lines represent the Observed, Original-simulated and Improved-simulated mixing ratios, respectively. The blue columns represent the relative differences (%) between Original and Improved simulations. The corresponding monitoring networks are (a) EMEP, (b) EPA, (c) CNEMC and (d) EANET.

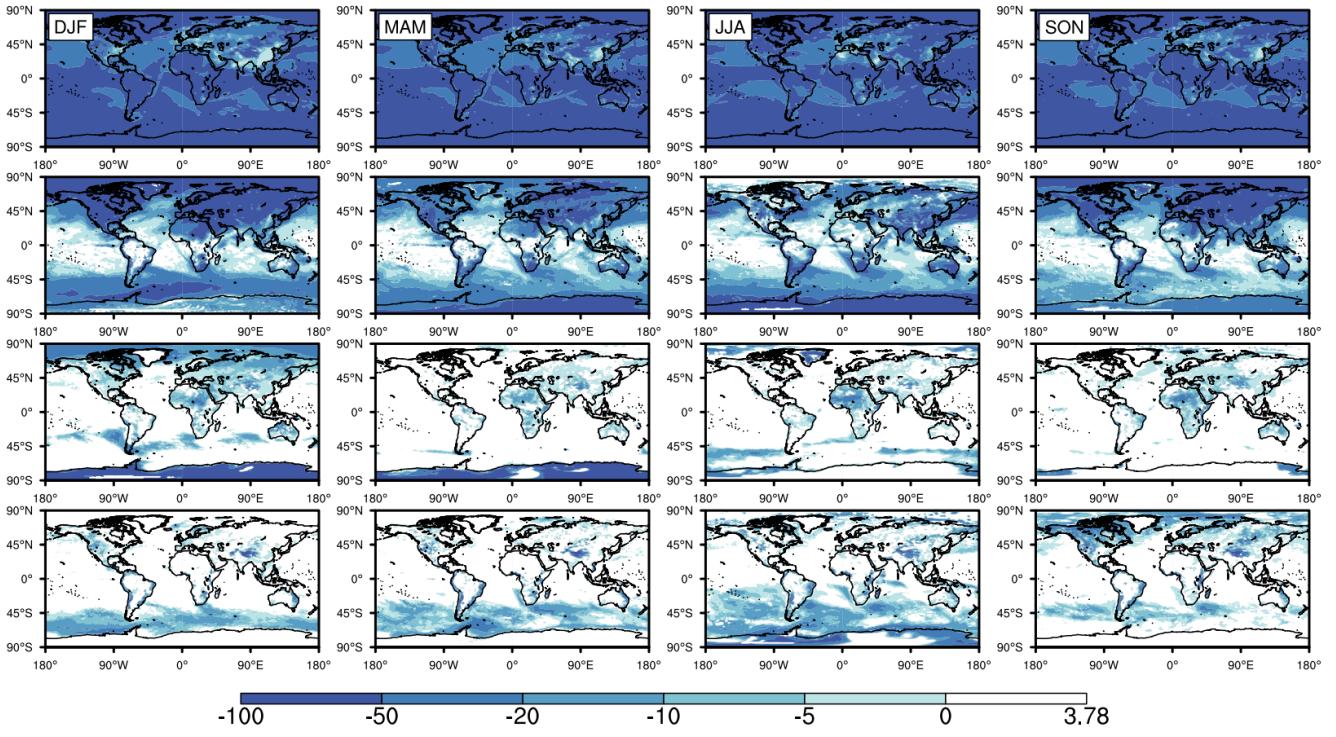


Figure S5: The relative differences (%) in global seasonally averaged surface SO₂ mixing ratios in 2015 with the incorporation of HO_x-chemistry, Fe-chemistry, N-chemistry and carbonate chemistry individually, from top to bottom (case 3~6 – case 1).

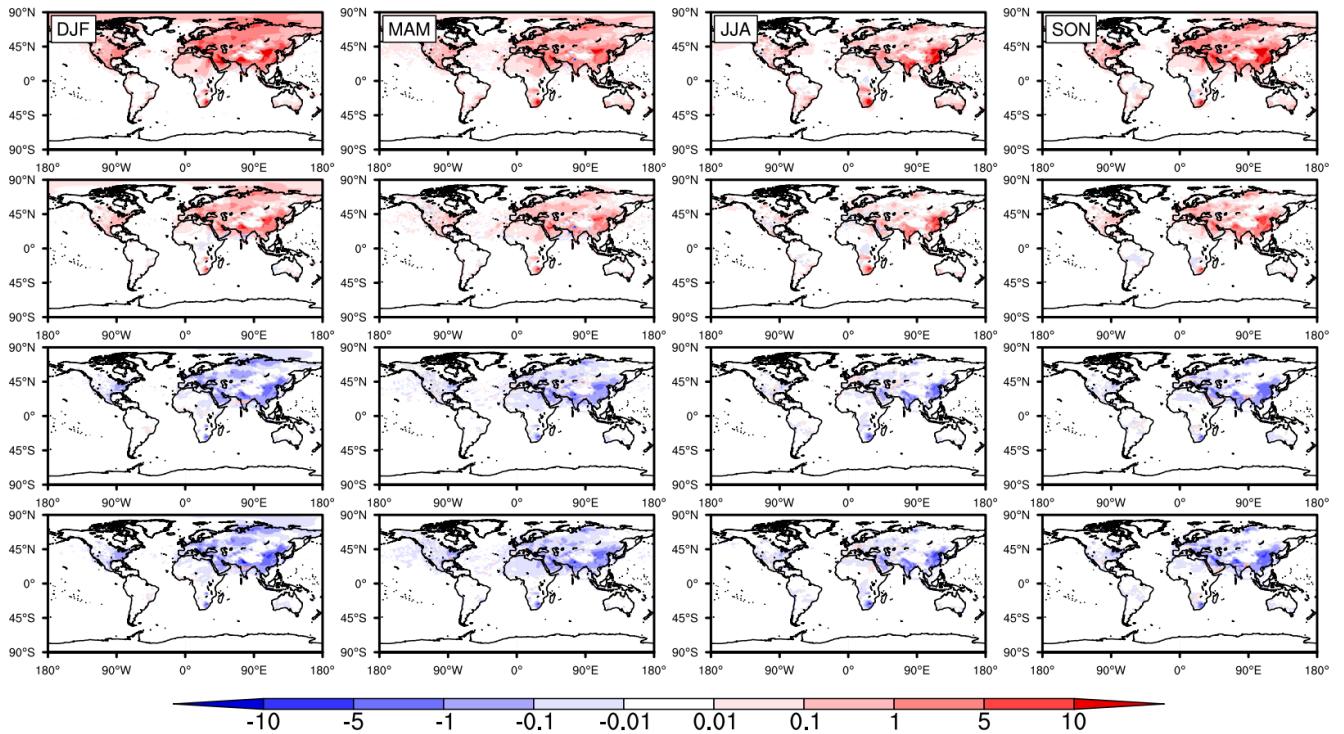


Figure S6: The differences in global seasonally averaged surface SO₂ mixing ratios (unit: ppbv) in 2015 after changing the soluble [Fe³⁺] concentration levels from 5 μM to 0.1 (top), 1, 20 and 100 μM (bottom) with the detailed aqueous-phase chemical mechanisms (case 7~10 – case 2).

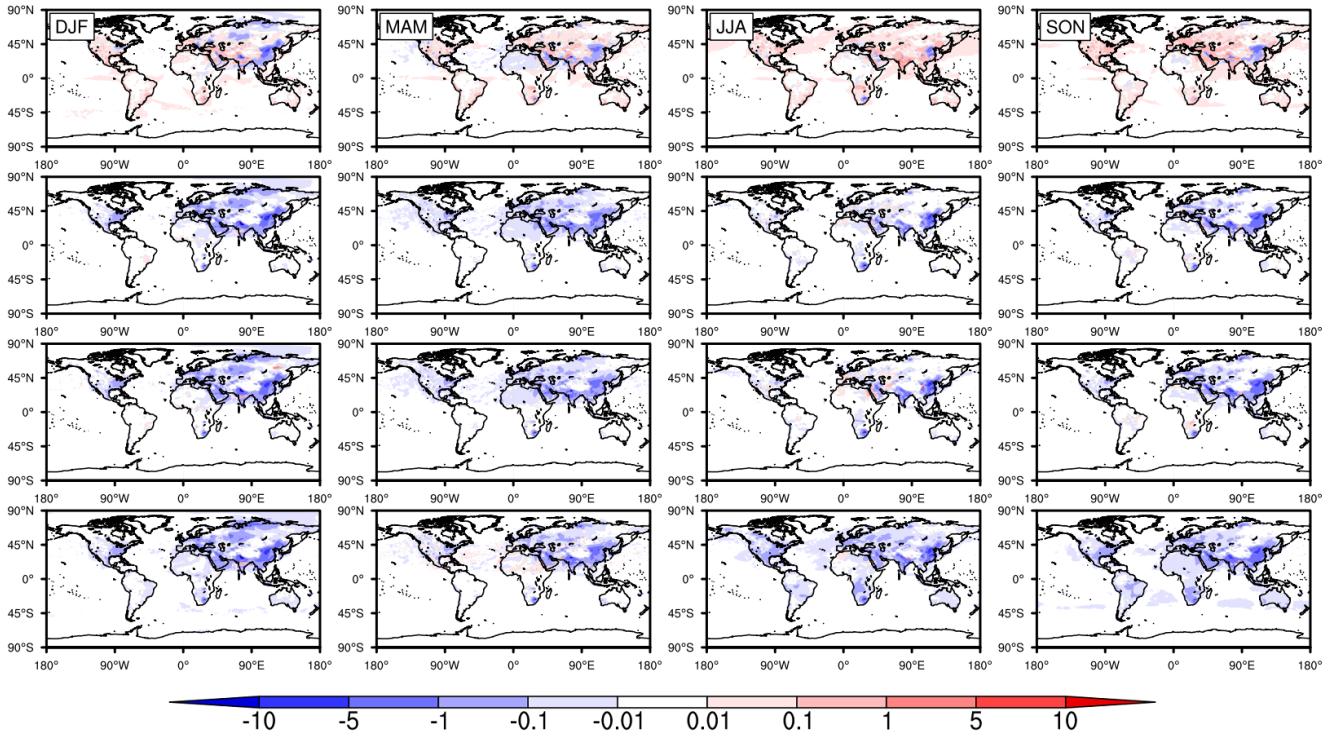


Figure S7: The differences in global seasonally averaged surface SO_2 mixing ratios (unit: ppbv) in 2015 at different pH values on the basis of the Improved case with the overall detailed in-cloud aqueous-phase chemical mechanisms (case 11~14 – case 2). The pH values from top to bottom are 3, 4, 5 and 6. $[\text{Fe}^{3+}]$ is set to $5 \mu\text{M}$.

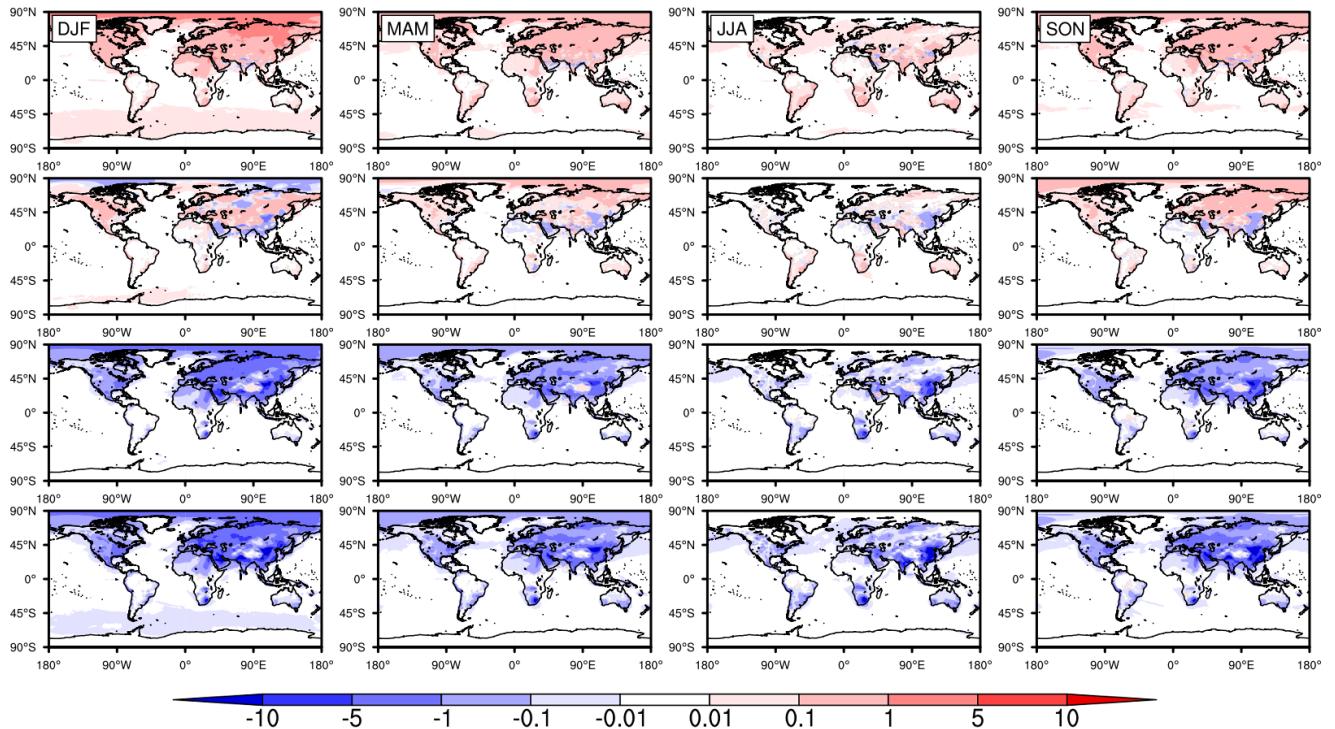


Figure S8: The differences in global seasonally averaged surface SO_2 mixing ratios (unit: ppbv) in 2015 at different pH values after the incorporation of N-chemistry individually (case 23~26 – case 5). The pH values from top to bottom are 3, 4, 5 and 6, respectively.

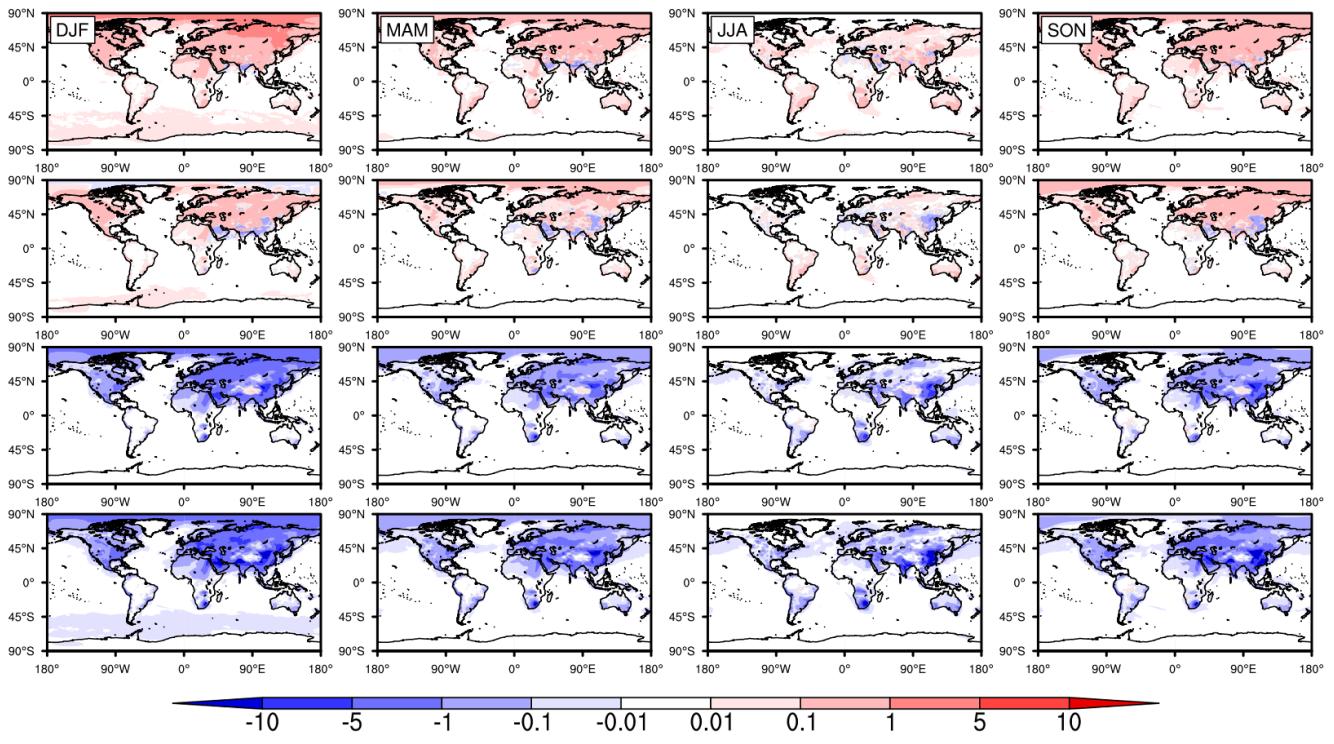


Figure S9: The differences in global seasonally averaged surface SO₂ mixing ratios (unit: ppbv) in 2015 at different pH values after the incorporation of HO_x-chemistry individually (case 15~18 – case 3). The pH values from top to bottom are 3, 4, 5 and 6, respectively.

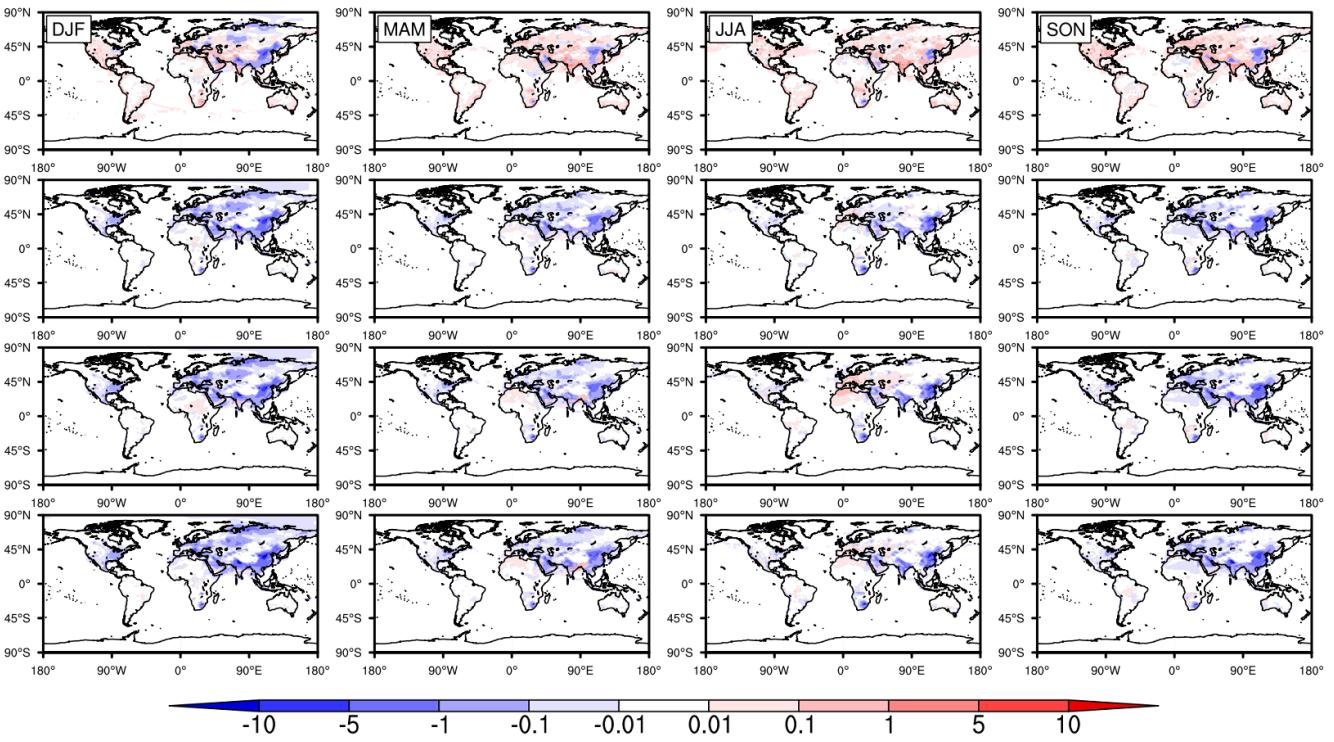


Figure S10: The differences in global seasonally averaged surface SO₂ mixing ratios (unit: ppbv) in 2015 at different pH values after the incorporation of Fe-chemistry individually (case 19~22 – case 4). The pH values from top to bottom are 3, 4, 5 and 6, respectively. [Fe³⁺] is set to 5 μ M.

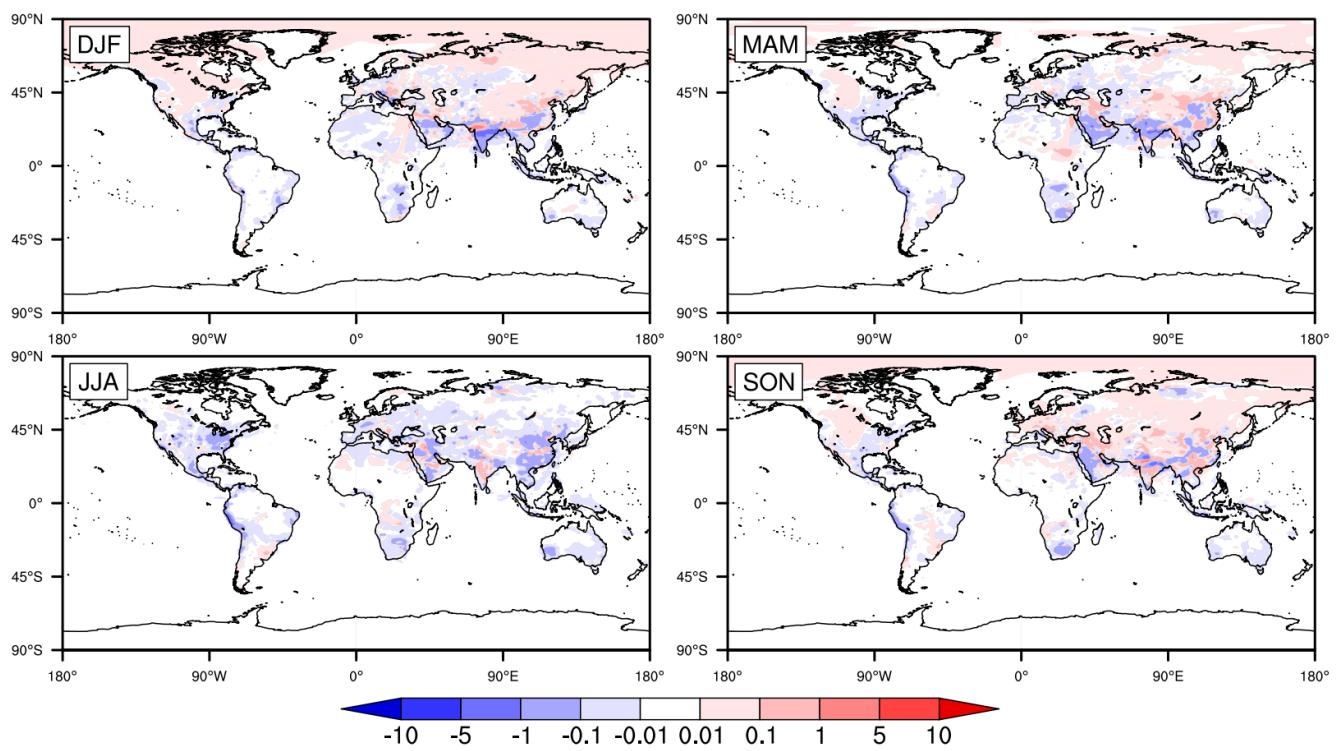


Figure S11: The differences in global seasonally averaged surface SO₂ mixing ratios (unit: ppbv) in 2015 with the incorporation of organic chemistry (case 27 – case 3).

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