



Supplement of

An advanced modelling study on the role of dimethyl sulfide in new particle formation in the pristine marine boundary layer

Robin Wollesen de Jonge et al.

Correspondence to: Robin Wollesen de Jonge (robin.wollesendejonge@helsinki.fi)

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Table S1. Gas-phase DMS reactions. Second order rate coefficients are given in units of $\text{cm}^3 \text{ molecules}^{-1} \text{ s}^{-1}$ and first order rate coefficients in units of s^{-1} .

Nr.	Reaction		Reaction Rate Coefficient	Ref.
G1	DMS + OH	$\rightarrow \text{CH}_3\text{SCH}_2\text{O}_2$	$1.12 \times 10^{-11} \times \exp(-250/T)$	[A]
G2	DMS + OH	$\rightarrow \text{CH}_3\text{SOHCH}_3$	KMT18	[B]
G3	DMS + NO_3	$\rightarrow \text{CH}_3\text{SCH}_2\text{O}_2 + \text{HNO}_3$	$1.9 \times 10^{-13} \times \exp(520/T)$	[A]
G4	DMS + Cl	$\rightarrow \text{CH}_3\text{SCH}_2\text{O}_2 + \text{HCl}$	$0.45 \times 3.4 \times 10^{-10}$	[B]
G5	DMS + Cl	$\rightarrow \text{CH}_3\text{SCH}_3\text{Cl}$	$0.55 \times 3.4 \times 10^{-10}$	[B]
G6	DMS + ClO	$\rightarrow \text{DMSO} + \text{Cl}$	$0.73 \times 1.7 \times 10^{-15} \times \exp(340/T)$	[B]
G7	DMS + ClO	$\rightarrow \text{CH}_3\text{SCH}_2\text{O}_2 + \text{HOCl}$	$0.27 \times 1.7 \times 10^{-15} \times \exp(340/T)$	[B]
G8	DMS + Cl ₂	$\rightarrow \text{CH}_3\text{SCH}_2\text{Cl} + \text{HCl}$	3.4×10^{-14}	[B]
G9	DMS + Br	$\rightarrow \text{CH}_3\text{SCH}_2\text{O}_2 + \text{HBr}$	$9 \times 10^{-11} \times \exp(-2390/T)$	[B]
G10	DMS + Br	$\rightarrow \text{CH}_3\text{SCH}_3\text{Br}$	KMT54	[B]
G11	DMS + BrO	$\rightarrow \text{DMSO} + \text{Br}$	$1.5 \times 10^{-14} \times \exp(1000/T)$	[B]
G12	DMS + IO	$\rightarrow \text{DMSO} + \text{I}$	$3.3 \times 10^{-13} \times \exp(-925/T)$	[B]
G13	$\text{CH}_3\text{SOHCH}_3$	$\rightarrow \text{DMS} + \text{OH}$	$(1.7 \times 10^{-42} \times [\text{O}_2] \times \exp(7810/T))$ $/((1+5.5 \times 10^{-31} \times [\text{O}_2] \times \exp(7640/T)))$ $/((8.3 \times 10^{-29} \times T \times \exp(5136/T)))$	[B]
G14	$\text{CH}_3\text{SOHCH}_3$	$\rightarrow \text{HODMSO}_2$	$8.5 \times 10^{-13} \times [\text{O}_2]$	[B]
G15	$\text{CH}_3\text{SOHCH}_3$	$\rightarrow \text{CH}_3\text{SOH} + \text{CH}_3\text{O}_2$	5×10^5	[B]
G16	$\text{CH}_3\text{SOH} + \text{OH}$	$\rightarrow \text{CH}_3\text{SO}$	5×10^{-11}	[B]
G17	$\text{CH}_3\text{SCH}_2\text{Cl} + \text{OH}$	$\rightarrow \text{CH}_3\text{SOH} + \text{CH}_2\text{ClO}_2$	2.5×10^{-12}	[B]
G18	$\text{CH}_3\text{SCH}_3\text{Cl} + \text{NO}_2$	$\rightarrow \text{DMS} + \text{ClNO}_2$	2.7×10^{-11}	[B]
G19	$\text{CH}_3\text{SCH}_3\text{Cl} + \text{NO}$	$\rightarrow \text{DMS} + \text{ClNO}$	1.2×10^{-11}	[B]
G20	$\text{CH}_3\text{SCH}_3\text{Cl}$	$\rightarrow \text{DMSO} + \text{ClO}$	$4 \times 10^{-18} \times [\text{O}_2]$	[B]
G21	$\text{CH}_3\text{SCH}_3\text{Cl}$	$\rightarrow \text{DMS} + \text{Cl}$	9×10^1	[B]
G22	$\text{CH}_3\text{SOCH}_3\text{Cl}$	$\rightarrow \text{DMSO}_2 + \text{ClO}$	$3 \times 10^{-18} \times [\text{O}_2]$	[B]
G23	$\text{CH}_3\text{SOCH}_3\text{Cl} + \text{NO}$	$\rightarrow \text{DMSO} + \text{ClNO}$	1.2×10^{-11}	[B]
G24	$\text{CH}_3\text{SOCH}_3\text{Cl} + \text{NO}_2$	$\rightarrow \text{DMSO} + \text{ClNO}_2$	2.1×10^{-11}	[B]
G25	$\text{CH}_3\text{SOCH}_3\text{Cl} + \text{CH}_3\text{SOCH}_3\text{Cl}$	$\rightarrow \text{DMSO} + \text{DMSO} + \text{Cl}_2$	3×10^{-11}	[B]
G26	$\text{CH}_3\text{SOCH}_3\text{Cl}$	$\rightarrow \text{DMSO} + \text{Cl}$	9×10^1	[B]
G27	$\text{CH}_3\text{SCH}_3\text{Br}$	$\rightarrow \text{DMSO} + \text{BrO}$	$1 \times 10^{-18} \times [\text{O}_2]$	[B]
G28	$\text{CH}_3\text{SCH}_3\text{Br}$	$\rightarrow \text{DMS} + \text{Br}$	1.02×10^4	[B]
G29	$\text{DMSO} + \text{BrO}$	$\rightarrow \text{DMSO}_2 + \text{Br}$	1×10^{-14}	[B]

Table S1. Gas-phase DMS reactions continued

Nr.	Reaction		Reaction Rate Coefficient	Ref.
G30	$\text{CH}_3\text{SCH}_2\text{O}_2$	$\rightarrow \text{OOCH}_2\text{SCH}_2\text{OOH}$	$2.2433 \times 10^{11} \times \exp(-9.8016 \times 10^3/T)$ $\times \exp(1.0348 \times 10^8/T^3) \times 2.75$	[C][D]
G31	$\text{OOCH}_2\text{SCH}_2\text{OOH}$	$\rightarrow \text{HPMTF} + \text{OH}$	$6.097 \times 10^{11} \times \exp(-9.4892 \times 10^3/T)$ $\times \exp(1.102 \times 10^8/T^3)$	[C]
G32	$\text{OOCH}_2\text{SCH}_2\text{OOH} + \text{NO}$	$\rightarrow \text{HOOCH}_2\text{S} + \text{NO}_2 + \text{HCHO}$	$4.9 \times 10^{-12} \times \exp(260/T)$	[C]
G33	$\text{OOCH}_2\text{SCH}_2\text{OOH} + \text{HO}_2$	$\rightarrow \text{HOOCH}_2\text{SCH}_2\text{OOH}$	$1.13 \times 10^{-13} \times \exp(1300/T)$	[C]
G34	$\text{HPMTF} + \text{OH}$	$\rightarrow \text{HOOCH}_2\text{SCO}$	2.1×10^{-11}	[D]
G35	HOOCH_2SCO	$\rightarrow \text{HOOCH}_2\text{S} + \text{CO}$	$9.2 \times 10^9 \times \exp(-505.4/T)$	[E]
G36	HOOCH_2SCO	$\rightarrow \text{HCHO} + \text{OH} + \text{OCS}$	$1.6 \times 10^7 \times \exp(-1468.6/T)$	[E]
G37	$\text{HOOCH}_2\text{S} + \text{O}_3$	$\rightarrow \text{HOOCH}_2\text{SO}$	$1.15 \times 10^{-12} \times \exp(430/T)$	[E]
G38	$\text{HOOCH}_2\text{S} + \text{NO}_2$	$\rightarrow \text{HOOCH}_2\text{SO} + \text{NO}$	$6.00 \times 10^{-11} \times \exp(240/T)$	[E]
G39	$\text{HOOCH}_2\text{SO} + \text{O}_3$	$\rightarrow \text{SO}_2 + \text{HCHO} + \text{OH}$	4.00×10^{-13}	[E]
G40	$\text{HOOCH}_2\text{SO} + \text{NO}_2$	$\rightarrow \text{SO}_2 + \text{HCHO} + \text{OH} + \text{NO}$	1.20×10^{-11}	[E]
G41	$\text{CH}_3\text{SOH} + \text{O}_3$	$\rightarrow \text{CH}_3\text{O}_2 + \text{HO}_2 + \text{SO}_2$	2×10^{-12}	[F]
G42	$\text{CH}_3\text{SCH}_2\text{O}_2 + \text{HO}_2$	$\rightarrow \text{CH}_3\text{SCH}_2\text{OOH}$	$\text{KRO}_2\text{HO}_2 \times 0.387$	[A]
G43	$\text{CH}_3\text{SCH}_2\text{O}_2 + \text{NO}$	$\rightarrow \text{CH}_3\text{SCH}_2\text{O} + \text{NO}_2$	$4.9 \times 10^{-12} \times \exp(260/T)$	[A]
G44	$\text{CH}_3\text{SCH}_2\text{O}_2 + \text{NO}_3$	$\rightarrow \text{CH}_3\text{SCH}_2\text{O} + \text{NO}_2$	KRO_2NO_3	[A]
G45	$\text{CH}_3\text{SCH}_2\text{O}_2$	$\rightarrow \text{CH}_3\text{SCH}_2\text{O}$	$3.74 \times 10^{-12} \times [\text{RO}_2] \times 0.8$	[A]
G46	$\text{CH}_3\text{SCH}_2\text{O}_2$	$\rightarrow \text{CH}_3\text{SCH}_2\text{OH}$	$3.74 \times 10^{-12} \times [\text{RO}_2] \times 0.1$	[A]
G47	$\text{CH}_3\text{SCH}_2\text{O}_2$	$\rightarrow \text{CH}_3\text{SCHO}$	$3.74 \times 10^{-12} \times [\text{RO}_2] \times 0.1$	[A]
G48	$\text{HODMSO}_2 + \text{NO}$	$\rightarrow \text{DMSO}_2 + \text{HO}_2 + \text{NO}_2$	KRO_2NO	[A]
G49	HODMSO_2	$\rightarrow \text{DMSO} + \text{HO}_2$	$8.90 \times 10^{10} \times \exp(-6040/T)$	[A]
G50	$\text{CH}_3\text{SCH}_2\text{OOH} + \text{OH}$	$\rightarrow \text{CH}_3\text{SCHO} + \text{OH}$	7.03×10^{-11}	[A]
G51	$\text{CH}_3\text{SCH}_2\text{OOH}$	$\rightarrow \text{CH}_3\text{SCH}_2\text{O} + \text{OH}$	J(41)	[A]
G52	$\text{CH}_3\text{SCH}_2\text{O}$	$\rightarrow \text{CH}_3\text{S} + \text{HCHO}$	KDEC	[A]
G53	$\text{CH}_3\text{SCH}_2\text{OH} + \text{OH}$	$\rightarrow \text{CH}_3\text{SCHO} + \text{HO}_2$	2.78×10^{-11}	[A]
G54	$\text{CH}_3\text{SCHO} + \text{OH}$	$\rightarrow \text{CH}_3\text{S} + \text{CO}$	1.11×10^{-11}	[A]
G55	CH_3SCHO	$\rightarrow \text{CH}_3\text{S} + \text{CO} + \text{HO}_2$	J(15)	[A]
G56	$\text{DMSO}_2 + \text{OH}$	$\rightarrow \text{DMSO}_2\text{O}_2$	4.40×10^{-14}	[A]
G57	$\text{DMSO} + \text{OH}$	$\rightarrow \text{MSIA} + \text{CH}_3\text{O}_2$	$6.10 \times 10^{-12} \times \exp(800/T)$	[A]
G58	$\text{DMSO} + \text{NO}_3$	$\rightarrow \text{DMSO}_2 + \text{NO}_2$	2.9×10^{-13}	[B]
G59	$\text{DMSO} + \text{Cl}$	$\rightarrow \text{CH}_3\text{SOCH}_2\text{O}_2 + \text{HCl}$	1.45×10^{-11}	[B]
G60	$\text{DMSO} + \text{Cl}$	$\rightarrow \text{CH}_3\text{SOCH}_2\text{Cl}$	7.4×10^{-11}	[B]
G61	$\text{CH}_3\text{SOCH}_2\text{O}_2 + \text{NO}$	$\rightarrow \text{CH}_3\text{SO} + \text{HCHO} + \text{NO}_2$	7.5×10^{-12}	[B]
G62	$\text{CH}_3\text{SOCH}_2\text{O}_2 + \text{HO}_2$	$\rightarrow \text{CH}_3\text{SOCH}_2\text{OOH}$	1.5×10^{-12}	[B]

Table S1. Gas-phase DMS reactions continued

Nr.	Reaction	Reaction Rate Coefficient	Ref.
G63	MSIA + OH $\rightarrow$ CH ₃ SO ₂	$4.3298 \times 10^{-12} \times \exp(904.2192/T)$	[G][H]
G64	MSIA + OH $\rightarrow$ HOMSIA	$9.6029 \times 10^{-13} \times \exp(825.0233/T)$	[G]
G65	HOMSIA $\rightarrow$ CH ₃ O ₂ + SO ₂	$1.7078 \times 10^{13} \times \exp(-1579.3/T)$	[G]
G66	HOMSIA $\rightarrow$ MSA + HO ₂	$1.4388 \times 10^{-15} \times \exp(6181.5.3/T) \times [\text{O}_2]$	[G]
G67	MSIA + NO ₃ $\rightarrow$ CH ₃ SO ₂ + HNO ₃	1×10^{-13}	[B]
G68	CH ₃ SOO + HO ₂ $\rightarrow$ CH ₃ SOOH	4×10^{-12}	[B]
G69	CH ₃ SOO $\rightarrow$ CH ₃ SO ₂	1	[B]
G70	CH ₃ SO ₂ + OH $\rightarrow$ MSA	5×10^{-11}	[B]
G71	CH ₃ SO ₂ + NO ₂ $\rightarrow$ CH ₃ SO ₃ + NO	2.2×10^{-11}	[B]
G72	CH ₃ S + NO ₂ $\rightarrow$ CH ₃ SO + NO	$6.00 \times 10^{-11} \times \exp(240/T)$	[A]
G73	CH ₃ S + O ₃ $\rightarrow$ CH ₃ SO	$1.15 \times 10^{-12} \times \exp(430/T)$	[A]
G74	CH ₃ S $\rightarrow$ CH ₃ SOO	$1.20 \times 10^{-16} \times \exp(1580/T) \times [\text{O}_2]$	[A]
G75	DMSO ₂ O ₂ + HO ₂ $\rightarrow$ DMSO ₂ OOH	KRO ₂ HO ₂ $\times$ 0.387	[A]
G76	DMSO ₂ O ₂ + NO $\rightarrow$ DMSO ₂ O + NO ₂	KRO ₂ NO	[A]
G77	DMSO ₂ O ₂ + NO ₃ $\rightarrow$ DMSO ₂ O + NO ₂	KRO ₂ NO ₃	[A]
G78	DMSO ₂ O ₂ $\rightarrow$ CH ₃ SO ₂ CHO	$2.00 \times 10^{-12} \times [\text{RO}_2] \times 0.2$	[A]
G79	DMSO ₂ O ₂ $\rightarrow$ DMSO ₂ O	$2.00 \times 10^{-12} \times [\text{RO}_2] \times 0.6$	[A]
G80	DMSO ₂ O ₂ $\rightarrow$ DMSO ₂ OH	$2.00 \times 10^{-12} \times [\text{RO}_2] \times 0.2$	[A]
G81	CH ₃ SO + NO ₂ $\rightarrow$ CH ₃ O ₂ + SO ₂ + NO	$1.20 \times 10^{-11} \times 0.25$	[A]
G82	CH ₃ SO + NO ₂ $\rightarrow$ CH ₃ SO ₂ + NO	$1.20 \times 10^{-11} \times 0.75$	[A]
G83	CH ₃ SO + O ₃ $\rightarrow$ CH ₃ O ₂ + SO ₂	4.00×10^{-13}	[A]
G84	CH ₃ SO $\rightarrow$ CH ₃ SOO ₂	$3.12 \times 10^{-16} \times \exp(1580/T) \times [\text{O}_2]$	[A]
G85	CH ₃ SOO + NO $\rightarrow$ CH ₃ SO + NO ₂	1.1×10^{-11}	[A]
G86	CH ₃ SOO + NO ₂ $\rightarrow$ CH ₃ SO + NO ₃	2.2×10^{-11}	[A]
G87	CH ₃ SOO $\rightarrow$ CH ₃ O ₂ + SO ₂	$5.60 \times 10^{16} \times \exp(-10870/T)$	[A]
G88	CH ₃ SOO $\rightarrow$ CH ₃ S	$3.50 \times 10^{10} \times \exp(-3560/T)$	[A]
G89	DMSO ₂ OOH + OH $\rightarrow$ CH ₃ SO ₂ CHO + OH	1.26×10^{-12}	[A]
G90	DMSO ₂ OOH + OH $\rightarrow$ DMSO ₂ O ₂	3.60×10^{-12}	[A]
G91	DMSO ₂ OOH $\rightarrow$ DMSO ₂ O + OH	J(41)	[A]
G92	DMSO ₂ O $\rightarrow$ CH ₃ SO ₂ + HCHO	KDEC	[A]
G93	CH ₃ SO ₂ CHO + OH $\rightarrow$ CH ₃ SO ₂ + CO	1.78×10^{-12}	[A]
G94	CH ₃ SO ₂ CHO $\rightarrow$ CH ₃ SO ₂ + CO + HO ₂	J(15)	[A]
G95	DMSO ₂ OH + OH $\rightarrow$ CH ₃ SO ₂ CHO + HO ₂	5.23×10^{-13}	[A]
G96	DMSO ₂ OH + OH $\rightarrow$ DMSO ₂ O	1.40×10^{-13}	[A]
G97	CH ₃ SO ₂ + O ₃ $\rightarrow$ CH ₃ SO ₃	3.00×10^{-13}	[A]

Table S1. Gas-phase DMS reactions continued

Nr.	Reaction		Reaction Rate Coefficient	Ref.
G98	CH_3SO_2	$\rightarrow \text{CH}_3\text{O}_2 + \text{SO}_2$	$5.00 \times 10^{13} \times \exp(-9673/T)$	[A]
G99	CH_3SO_2	$\rightarrow \text{CH}_3\text{SO}_2\text{O}_2$	$1.03 \times 10^{-16} \times \exp(1580/T) \times [\text{O}_2]$	[A]
G100	$\text{CH}_3\text{SOO}_2 + \text{HO}_2$	$\rightarrow \text{CH}_3\text{SO}_2 + \text{OH}$	$\text{KAPHO}_2 \times 0.44$	[A]
G101	$\text{CH}_3\text{SOO}_2 + \text{HO}_2$	$\rightarrow \text{CH}_3\text{SOOOH}$	$\text{KAPHO}_2 \times 0.41$	[A]
G102	$\text{CH}_3\text{SOO}_2 + \text{HO}_2$	$\rightarrow \text{MSIA} + \text{O}_3$	$\text{KAPHO}_2 \times 0.15$	[A]
G103	$\text{CH}_3\text{SOO}_2 + \text{NO}$	$\rightarrow \text{CH}_3\text{SO}_2 + \text{NO}_2$	1.00×10^{-11}	[A]
G104	$\text{CH}_3\text{SOO}_2 + \text{NO}_2$	$\rightarrow \text{CH}_3\text{SOO}_2\text{NO}_2$	$1.20 \times 10^{-12} \times (T/300)^{-0.9}$	[A]
G105	$\text{CH}_3\text{SOO}_2 + \text{NO}_3$	$\rightarrow \text{CH}_3\text{SO}_2 + \text{NO}_2$	$\text{KRO}_2\text{NO}_3 \times 1.74$	[A]
G106	CH_3SOO_2	$\rightarrow \text{CH}_3\text{SO}$	$9.10 \times 10^{10} \times \exp(-3560/T)$	[A]
G107	CH_3SOO_2	$\rightarrow \text{CH}_3\text{SO}_2$	$1.00 \times 10^{-11} \times [\text{RO}_2] \times 0.7$	[A]
G108	CH_3SOO_2	$\rightarrow \text{MSIA}$	$1.00 \times 10^{-11} \times [\text{RO}_2] \times 0.3$	[A]
G109	$\text{CH}_3\text{SO}_3 + \text{HO}_2$	$\rightarrow \text{MSA}$	5.00×10^{-11}	[A]
G110	$\text{CH}_3\text{SO}_3 + \text{DMS}$	$\rightarrow \text{MSA} + \text{CH}_3\text{SCH}_2\text{O}_2$	1.45×10^{-13}	[I][J]
G111	CH_3SO_3	$\rightarrow \text{CH}_3\text{O}_2 + \text{SO}_3$	$5.00 \times 10^{13} \times \exp(-9946/T)$	[A]
G112	$\text{CH}_3\text{SO}_2\text{O}_2 + \text{HO}_2$	$\rightarrow \text{CH}_3\text{SO}_2\text{OOH}$	$\text{KAPHO}_2 \times 0.41$	[A]
G113	$\text{CH}_3\text{SO}_2\text{O}_2 + \text{HO}_2$	$\rightarrow \text{CH}_3\text{SO}_3 + \text{OH}$	$\text{KAPHO}_2 \times 0.44$	[A]
G114	$\text{CH}_3\text{SO}_2\text{O}_2 + \text{HO}_2$	$\rightarrow \text{MSA} + \text{O}_3$	$\text{KAPHO}_2 \times 0.15$	[A]
G115	$\text{CH}_3\text{SO}_2\text{O}_2 + \text{NO}$	$\rightarrow \text{CH}_3\text{SO}_3 + \text{NO}_2$	1.00×10^{-11}	[A]
G116	$\text{CH}_3\text{SO}_2\text{O}_2 + \text{NO}_2$	$\rightarrow \text{CH}_3\text{SO}_4\text{NO}_2$	$1.20 \times 10^{-12} \times (T/300)^{-0.9}$	[A]
G117	$\text{CH}_3\text{SO}_2\text{O}_2 + \text{NO}_3$	$\rightarrow \text{CH}_3\text{SO}_3 + \text{NO}_2$	$\text{KRO}_2\text{NO}_3 \times 1.74$	[A]
G118	$\text{CH}_3\text{SO}_2\text{O}_2$	$\rightarrow \text{CH}_3\text{SO}_2$	$3.01 \times 10^{10} \times \exp(-3560/T)$	[A]
G119	$\text{CH}_3\text{SO}_2\text{O}_2$	$\rightarrow \text{CH}_3\text{SO}_3$	$1.00 \times 10^{-11} \times [\text{RO}_2] \times 0.7$	[A]
G120	$\text{CH}_3\text{SO}_2\text{O}_2$	$\rightarrow \text{MSA}$	$1.00 \times 10^{-11} \times [\text{RO}_2] \times 0.3$	[A]
G121	$\text{CH}_3\text{SOOOH} + \text{OH}$	$\rightarrow \text{CH}_3\text{SOO}_2$	9.00×10^{-11}	[A]
G122	CH_3SOOOH	$\rightarrow \text{CH}_3\text{SO}_2 + \text{OH}$	J(41)	[A]
G123	$\text{CH}_3\text{SOO}_2\text{NO}_2 + \text{OH}$	$\rightarrow \text{MSIA} + \text{NO}_2$	1.00×10^{-11}	[A]
G124	$\text{CH}_3\text{SOO}_2\text{NO}_2$	$\rightarrow \text{CH}_3\text{SOO}_2 + \text{NO}_2$	$5.40 \times 10^{16} \times \exp(-13112/T)$	[A]

[A] MCMv3.1.1, [B] Hoffmann et al. (2016), [C] Veres et al. (2020), [D] Ye et al. (2022), [E] Wu et al. (2014), [F] Berndt et al. (2020), [G] This work, [H] Kukui et al. (2003), [I] Yin et al. (1990), [J] Jacob et al. (2024)

Table S2. Aqueous-phase DMS reactions. Second order rate coefficients are given in units of $\text{L mol}^{-1} \text{s}^{-1}$ and first order rate coefficients in units of s^{-1} .

Nr.	Reaction	Reaction Rate Coefficient	Ref.
A1	$\text{DMS} + \text{O}_3 \rightarrow \text{DMSO}$	$8.61 \times 10^8 \times \exp(-2600 \times (1/T-1/298));$	[B]
A2	$\text{DMS} + \text{OH} \rightarrow \text{DMSO} + \text{HO}_2$	1.9×10^{10}	[B]
A3	$\text{DMS} + \text{Cl}_2^- \rightarrow \text{CH}_3\text{SCH}_3\text{Cl} + \text{Cl}^-$	3×10^9	[B]
A4	$\text{DMS} + \text{Br}_2^- \rightarrow \text{CH}_3\text{SCH}_3\text{Br} + \text{Br}^-$	3.2×10^9	[B]
A5	$\text{DMS} + \text{H}_2\text{O}_2 \rightarrow \text{DMSO}$	3.4×10^{-2}	[B]
A6	$\text{CH}_3\text{SCH}_3\text{Cl} + \text{O}_2 \rightarrow \text{DMSO} + \text{ClO}$	2.41×10^3	[B]
A7	$\text{CH}_3\text{SCH}_3\text{Br} + \text{O}_2 \rightarrow \text{DMSO} + \text{BrO}$	6.02×10^2	[B]
A8	$\text{DMSO} + \text{O}_3 \rightarrow \text{DMSO}_2$	3×10^0	[B]
A9	$\text{DMSO} + \text{OH} \rightarrow \text{MSIA}$	$6.65 \times 10^9 \times \exp(-1270 \times (1/T-1/298))$	[B]
A10	$\text{DMSO} + \text{SO}_4^- \rightarrow \text{DMSO}^+ + \text{SO}_4^{2-}$	$2.97 \times 10^9 \times \exp(-1440 \times (1/T-1/298))$	[B]
A11	$\text{DMSO} + \text{Cl} \rightarrow \text{CH}_3\text{SOCH}_3\text{Cl}$	6.3×10^9	[B]
A12	$\text{DMSO} + \text{Cl}_2^- \rightarrow \text{CH}_3\text{SOCH}_3\text{Cl} + \text{Cl}^-$	1.6×10^7	[B]
A13	$\text{DMSO} + \text{H}_2\text{O}_2 \rightarrow \text{DMSO}_2$	2.75×10^{-6}	[B]
A14	$\text{DMSO}_{\text{ion}} + \text{Br}^- \rightarrow \text{CH}_3\text{SOCH}_3\text{Br}$	5×10^9	[B]
A15	$\text{CH}_3\text{SOCH}_3\text{Br} + \text{Br}^- \rightarrow \text{DMSO} + \text{Br}_2^-$	2.6×10^8	[B]
A16	$\text{CH}_3\text{SOCH}_3\text{Cl} \rightarrow \text{MSIA} + \text{HCl}$	$55.6 \times 1 \times 10^7$	[B]
A17	$\text{CH}_3\text{SOCH}_3\text{OH} \rightarrow \text{MSIA}$	1×10^7	[B]
A18	$\text{DMSO}_2 + \text{OH} \rightarrow \text{CH}_3\text{SO}_2\text{CH}_2$	$1.77 \times 10^7 \times \exp(-1690 \times (1/T-1/298))$	[B]
A19	$\text{DMSO}_2 + \text{SO}_4^- \rightarrow \text{CH}_3\text{SO}_2\text{CH}_2 + \text{SO}_4^{2-}$	$3.95 \times 10^6 \times \exp(-1360 \times (1/T-1/298))$	[B]
A20	$\text{DMSO}_2 + \text{Cl} \rightarrow \text{CH}_3\text{SO}_2\text{CH}_2 + \text{HCl}$	8.2×10^5	[B]
A21	$\text{DMSO}_2 + \text{Cl}_2^- \rightarrow \text{CH}_3\text{SO}_2\text{CH}_2 + \text{HCl} + \text{Cl}^-$	8.24×10^3	[B]
A22	$\text{DMSO}_2 + \text{O}_2 \rightarrow \text{CH}_3\text{SO}_2\text{CH}_2\text{O}_2$	2×10^9	[B]
A23	$\text{MSIA} + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3\text{H}$	3.5×10^7	[B]
A24	$\text{MSIA} + \text{OH} \rightarrow \text{CH}_3\text{SO}_3\text{H}_2$	6×10^9	[B]
A25	$\text{CH}_3\text{SO}_2^- + \text{OH} \rightarrow \text{CH}_3\text{SO}_2$	$0.9 \times 1.2 \times 10^{10}$	[B]
A26	$\text{CH}_3\text{SO}_2^- + \text{OH} \rightarrow \text{HSO}_3^-$	$0.1 \times 1.2 \times 10^{10}$	[B]
A27	$\text{CH}_3\text{SO}_2^- + \text{SO}_4^- \rightarrow \text{CH}_3\text{SO}_2 + \text{SO}_4^{2-}$	1×10^9	[B]
A28	$\text{CH}_3\text{SO}_2^- + \text{Cl}_2^- \rightarrow \text{CH}_3\text{SO}_2 + \text{Cl}^- + \text{Cl}^-$	8×10^8	[B]
A29	$\text{CH}_3\text{SO}_2^- + \text{H}_2\text{O}_2 \rightarrow \text{CH}_3\text{SO}_3^-$	1.2×10^{-2}	[B]
A30	$\text{CH}_3\text{SO}_2^- + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3^-$	2×10^6	[B]

Table S2. Aqueous-phase DMS reactions continued

Nr.	Reaction			Reaction Rate Coefficient	Ref.
A31	$\text{CH}_3\text{SO}_3\text{H}_2 + \text{O}_2$	$\rightarrow$	$\text{CH}_3\text{SO}_3\text{H} + \text{HO}_2$	1.2×10^9	[B]
A32	$\text{CH}_3\text{SO}_3\text{H} + \text{OH}$	$\rightarrow$	$\text{CH}_2\text{SO}_3\text{H}$	1.5×10^7	[B]
A33	$\text{CH}_3\text{SO}_3^- + \text{OH}$	$\rightarrow$	CH_2SO_3^-	$1.29 \times 10^7 \times \exp(-2630 \times (1/T-1/298))$	[B]
A34	$\text{CH}_3\text{SO}_3^- + \text{SO}_4^{2-}$	$\rightarrow$	$\text{CH}_3\text{SO}_3 + \text{SO}_4^{2-}$	$1.13 \times 10^4 \times \exp(-2490 \times (1/T-1/298))$	[B]
A35	$\text{CH}_3\text{SO}_3^- + \text{Cl}$	$\rightarrow$	$\text{CH}_3\text{SO}_3 + \text{Cl}^-$	4.9×10^5	[B]
A36	$\text{CH}_3\text{SO}_3^- + \text{Cl}_2^-$	$\rightarrow$	$\text{CH}_3\text{SO}_3 + \text{Cl}^- + \text{Cl}^-$	3.89×10^3	[B]
A37	$\text{CH}_3\text{SO}_2 + \text{OH}$	$\rightarrow$	$\text{CH}_3\text{SO}_3\text{H}$	1×10^{10}	[B]
A38	$\text{CH}_3\text{SO}_2 + \text{O}_3$	$\rightarrow$	CH_3SO_3	1.5×10^9	[B]
A39	$\text{CH}_3\text{SO}_2 + \text{SO}_3^{2-}$	$\rightarrow$	$\text{CH}_3\text{SO}_2^- + \text{SO}_4^{2-}$	1.7×10^9	[B]
A40	CH_3SO_2	$\rightarrow$	SO_2	8.3×10^4	[B]
A41	$\text{CH}_3\text{SO}_2 + \text{O}_2$	$\rightarrow$	$\text{CH}_3\text{SO}_2\text{O}_2$	1.2×10^9	[B]
A42	$\text{CH}_3\text{SO}_2 + \text{CH}_3\text{SO}_2$	$\rightarrow$	$\text{MSIA} + \text{CH}_3\text{SO}_3\text{H}$	8×10^8	[B]
A43	$\text{CH}_3\text{SO}_2\text{O}_2 + \text{CH}_3\text{SO}_2^-$	$\rightarrow$	$\text{CH}_3\text{SO}_3^- + \text{CH}_3\text{SO}_3$	6.2×10^8	[B]
A44	$\text{CH}_3\text{SO}_3 + \text{CH}_3\text{SO}_2^-$	$\rightarrow$	$\text{CH}_3\text{SO}_3^- + \text{CH}_3\text{SO}_2$	1×10^8	[B]
A45	CH_3SO_3	$\rightarrow$	SO_3	8.3×10^4	[B]
A46	$\text{CH}_3\text{SO}_3 + \text{HO}_2$	$\rightarrow$	$\text{CH}_3\text{SO}_3\text{H}$	8.3×10^5	[B]
A47	$\text{CH}_2\text{SO}_3\text{H} + \text{O}_2$	$\rightarrow$	$\text{O}_2\text{CH}_2\text{SO}_3\text{H}$	2×10^9	[B]
A48	$\text{CH}_2\text{SO}_3^- + \text{O}_2$	$\rightarrow$	$\text{O}_2\text{CH}_2\text{SO}_3^-$	2×10^9	[B]
A49	$\text{O}_2\text{CH}_2\text{SO}_3^-$	$\rightarrow$	$\text{HCHO} + \text{SO}_3^-$	$[\text{H}^+] \times 7 \times 10^3$	[B]

[B] Hoffmann et al. (2016)

S2 Alternative reaction rate coefficients

Table S3. Alternative reaction rate coefficients for key reactions. The study from which the rate coefficient used in the mechanism presented here was obtained is indicated in bold. Second order rate coefficients are given in units of $\text{cm}^3 \text{ molecules}^{-1} \text{ s}^{-1}$ and first order rate coefficients in units of s^{-1} .

Nr.	Reaction	Reaction Rate Coefficient	Ref.
G30	$\text{CH}_3\text{SCH}_2\text{O}_2 \rightarrow \text{OOCH}_2\text{SCH}_2\text{OOH}$	0.13 ± 0.03 (295K) 0.047 (295K) 0.23 ± 0.12 (295K)	Ye et al. (2022) Veres et al. (2020) Berndt et al. (2019)
G34	$\text{HPMTF} + \text{OH} \rightarrow \text{HOOCH}_2\text{SCO}$	2.1×10^{-11} 1.4×10^{-12}	Ye et al. (2022) Wu et al. (2014)
G64	$\text{MSIA} + \text{OH} \rightarrow \text{HOMSIA}$	1.53×10^{-11} (298K) 9.0×10^{-11} (298K)	This study Ye et al. (2022)
G98	$\text{CH}_3\text{SO}_2 \rightarrow \text{CH}_3\text{O}_2 + \text{SO}_2$	0.29 (295K) 6.0 (295K) 20.0 (295K)	MCMv3.3.1 Jacob et al. (2024) Berndt et al. (2024)
G111	$\text{CH}_3\text{SO}_3 \rightarrow \text{CH}_3\text{O}_2 + \text{SO}_3$	0.11 (295K) 9.71 (295K)	MCMv3.3.1 Cao et al. (2013)

S3 Mean source flux of key DMS oxidation products

Table S4. Mean H₂SO₄, MSA, SO₂, MSIA, DMSO, and HPMTF source flux during clear sky conditions of simulation days three to six for the sensitivity runs TEMP, WS, PRCP, SST, DMS, NH_x, and CLOUD.

Simulation	Sens. Run	Mean clear sky source flux (cm ⁻³ s ⁻¹)					
		H ₂ SO ₄	MSA	SO ₂	MSIA	DMSO	HPMTF
TEMP	273K	2.3×10 ³	2.3×10 ³	0.9×10 ⁴	2.6×10 ⁴	3.0×10 ⁴	1.2×10 ⁴
	278K	4.0×10 ³	2.7×10 ³	1.4×10 ⁴	2.7×10 ⁴	2.9×10 ⁴	1.7×10 ⁴
	283K	5.8×10 ³	2.9×10 ³	2.0×10 ⁴	2.5×10 ⁴	2.7×10 ⁴	2.1×10 ⁴
	288K	6.5×10 ³	2.7×10 ³	2.7×10 ⁴	2.1×10 ⁴	2.2×10 ⁴	2.7×10 ⁴
	293K	6.2×10 ³	2.3×10 ³	3.4×10 ⁴	1.8×10 ⁴	1.9×10 ⁴	3.2×10 ⁴
WS	2 m/s	2.0×10 ³	0.8×10 ³	0.6×10 ⁴	0.4×10 ⁴	0.4×10 ⁴	0.6×10 ⁴
	4 m/s	4.1×10 ³	1.9×10 ³	1.3×10 ⁴	1.1×10 ⁴	1.2×10 ⁴	1.4×10 ⁴
	6 m/s	5.8×10 ³	2.9×10 ³	2.0×10 ⁴	2.5×10 ⁴	2.7×10 ⁴	2.1×10 ⁴
	8 m/s	7.1×10 ³	3.7×10 ³	2.3×10 ⁴	5.4×10 ⁴	6.1×10 ⁴	2.5×10 ⁴
	10 m/s	7.6×10 ³	3.9×10 ³	2.3×10 ⁴	1.1×10 ⁵	1.3×10 ⁵	2.3×10 ⁴
PRCP	2.5 mm/h	5.5×10 ³	2.7×10 ³	2.0×10 ⁴	2.7×10 ⁴	2.8×10 ⁴	2.1×10 ⁴
	5 mm/h	5.7×10 ³	2.8×10 ³	2.0×10 ⁴	2.6×10 ⁴	2.7×10 ⁴	2.1×10 ⁴
	10 mm/h	5.8×10 ³	2.9×10 ³	2.0×10 ⁴	2.5×10 ⁴	2.7×10 ⁴	2.1×10 ⁴
	15 mm/h	5.8×10 ³	2.9×10 ³	2.0×10 ⁴	2.5×10 ⁴	2.6×10 ⁴	2.1×10 ⁴
SST	278K	5.2×10 ³	2.5×10 ³	1.8×10 ⁴	1.9×10 ⁴	2.0×10 ⁴	1.9×10 ⁴
	283K	5.8×10 ³	2.9×10 ³	2.0×10 ⁴	2.5×10 ⁴	2.7×10 ⁴	2.1×10 ⁴
	288K	6.4×10 ³	3.3×10 ³	2.1×10 ⁴	3.1×10 ⁴	3.4×10 ⁴	2.3×10 ⁴
	293K	6.9×10 ³	3.6×10 ³	2.3×10 ⁴	3.8×10 ⁴	4.2×10 ⁴	2.5×10 ⁴
DMS	5 nM	3.4×10 ³	1.5×10 ³	1.1×10 ⁴	1.3×10 ⁴	1.4×10 ⁴	1.1×10 ⁴
	10 nM	5.8×10 ³	2.9×10 ³	2.0×10 ⁴	2.5×10 ⁴	2.7×10 ⁴	2.1×10 ⁴
	15 nM	7.3×10 ³	4.0×10 ³	2.7×10 ⁴	3.4×10 ⁴	3.7×10 ⁴	3.1×10 ⁴
	20 nM	8.3×10 ³	5.0×10 ³	3.3×10 ⁴	4.2×10 ⁴	4.5×10 ⁴	4.0×10 ⁴
NH _x	0.1 mmol/m ³	5.6×10 ³	2.8×10 ³	2.0×10 ⁴	2.2×10 ⁴	2.3×10 ⁴	2.2×10 ⁴
	0.2 mmol/m ³	5.7×10 ³	2.8×10 ³	2.0×10 ⁴	2.3×10 ⁴	2.5×10 ⁴	2.2×10 ⁴
	0.3 mmol/m ³	5.8×10 ³	2.9×10 ³	2.0×10 ⁴	2.5×10 ⁴	2.7×10 ⁴	2.1×10 ⁴
	0.4 mmol/m ³	5.9×10 ³	2.9×10 ³	2.0×10 ⁴	2.6×10 ⁴	2.8×10 ⁴	2.1×10 ⁴
CLOUD	No Clouds	5.8×10 ³	2.9×10 ³	2.0×10 ⁴	2.5×10 ⁴	2.7×10 ⁴	2.1×10 ⁴
	Clouds	2.5×10 ³	1.3×10 ³	1.8×10 ⁴	1.5×10 ⁴	2.4×10 ⁴	2.0×10 ⁴

S4 Quantum chemical calculations

The schematic potential energy surfaces (PESs) for the reactions of MSIA with OH are shown in Figure S1.1. Two reaction pathways were identified: H-abstraction and OH-addition. For the H-abstraction channel, OH can abstract either the hydrogen atom from the S-OH group or from the methyl group of MSIA. Two transition-state conformations (TS_{abs-1} and TS_{abs-3}) were found for abstraction from the S-OH site, corresponding to different energy barriers, while TS_{abs-2} corresponds to abstraction from the methyl group. The most favourable H-abstraction pathway proceeds via TS_{abs-1} , which is stabilized by a pre-reaction complex involving two hydrogen bonds between MSIA and OH. The calculated barrier height for TS_{abs-1} is 7.1 kcal mol⁻¹. For the OH-addition reaction, a single transition state (TS_{add}) was identified, with a barrier of 5.8 kcal mol⁻¹.

The fate of the OH-addition intermediate IM_{add} (or HOMSIA as referred to in the main text) was also investigated. Earlier studies suggested that IM_{add} undergoes rapid S-C bond cleavage to form H₂SO₃ and a CH₃ radical (Lv et al., 2019; Gonzalez-García et al., 2007). Our results, however, indicate that IM_{add} can also react with O₂ to produce MSA and HO₂. The calculated unimolecular dissociation rate of IM_{add} is 8.5×10^{10} s⁻¹, while the pseudo-first-order rate constant for the O₂-assisted H-abstraction pathway is 7.3×10^{12} s⁻¹ (based on a bimolecular rate constant of 1.47×10^{-6} cm³ molecules⁻¹ s⁻¹ and an O₂ concentration of 5×10^{18} molecules cm⁻³). This additional pathway provides a previously uninvestigated source of MSA formation in the atmosphere.

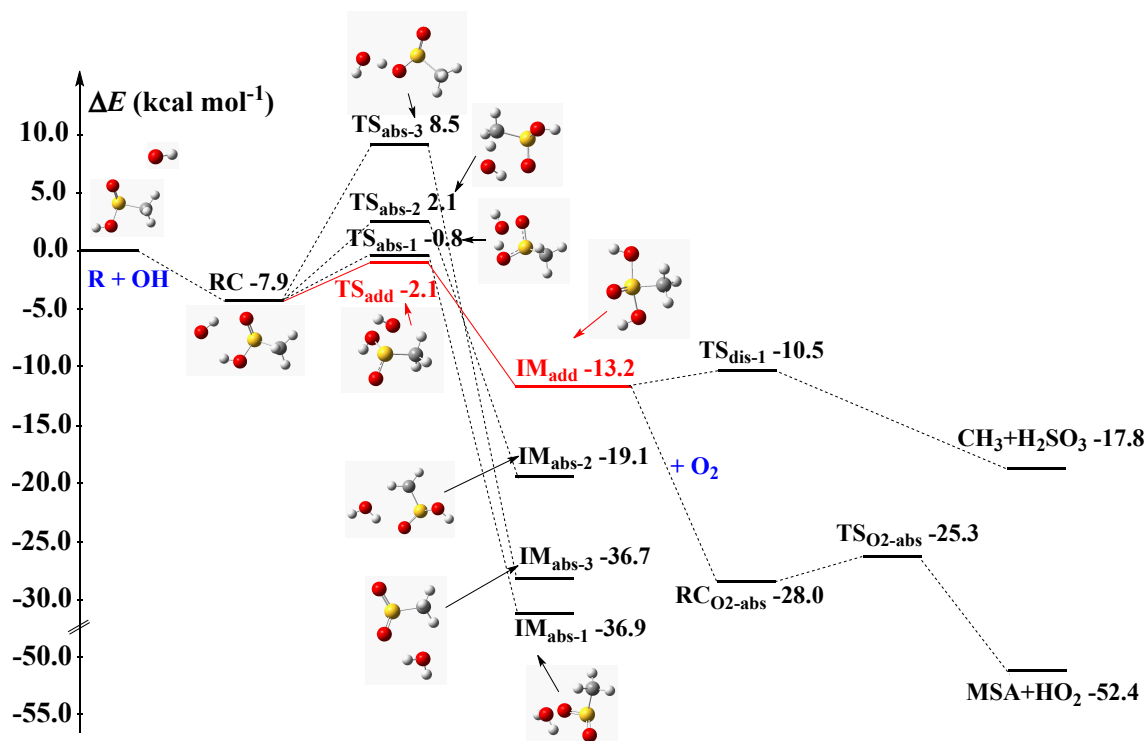


Figure S1. Schematic potential energy surfaces for the reactions of MSIA and OH at the F12a//M06-2X/6-311+G(3df,2p) level of theory.

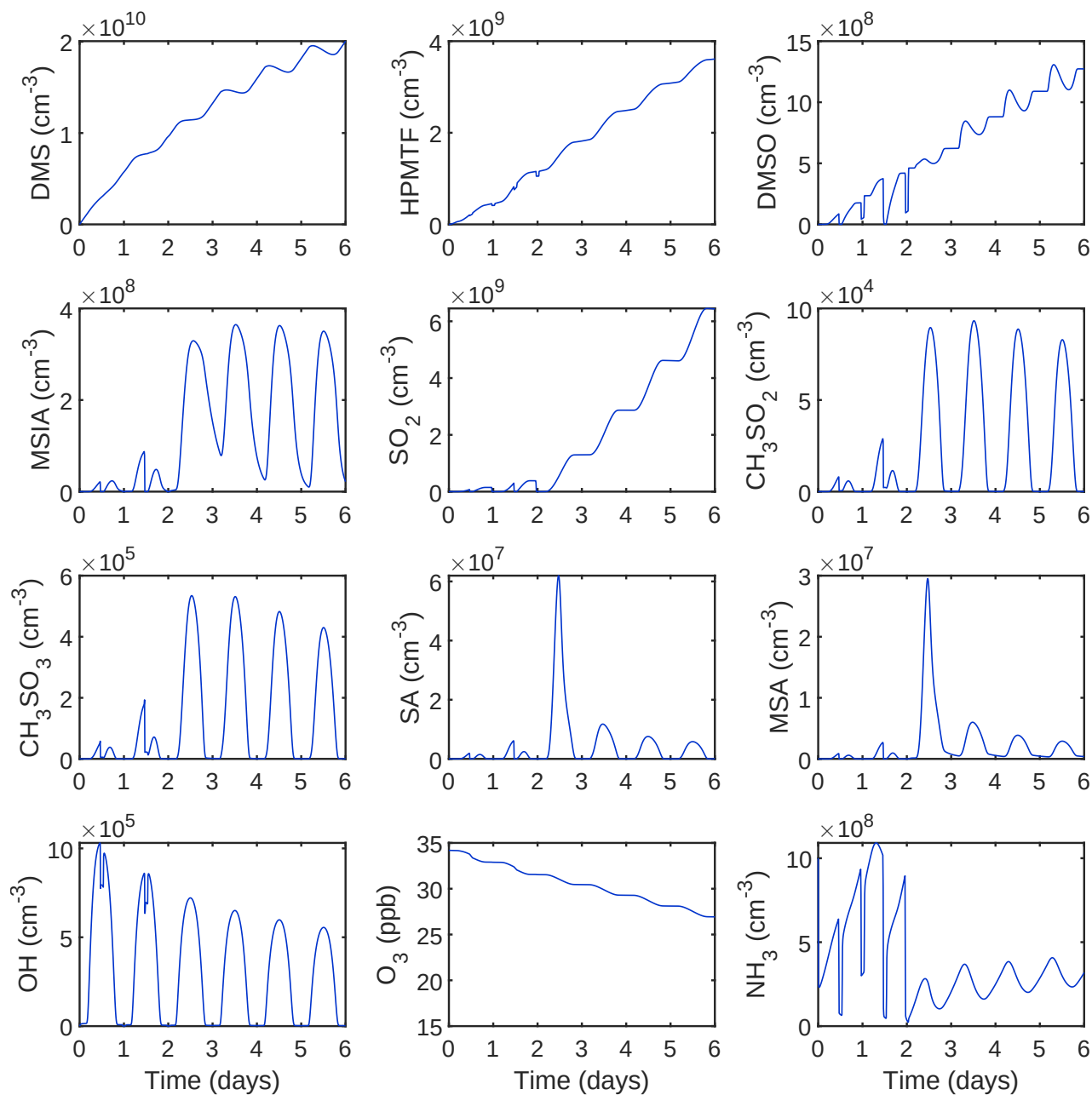


Figure S2. Concentrations of key gas-phase species in the BaseCase Simulation.

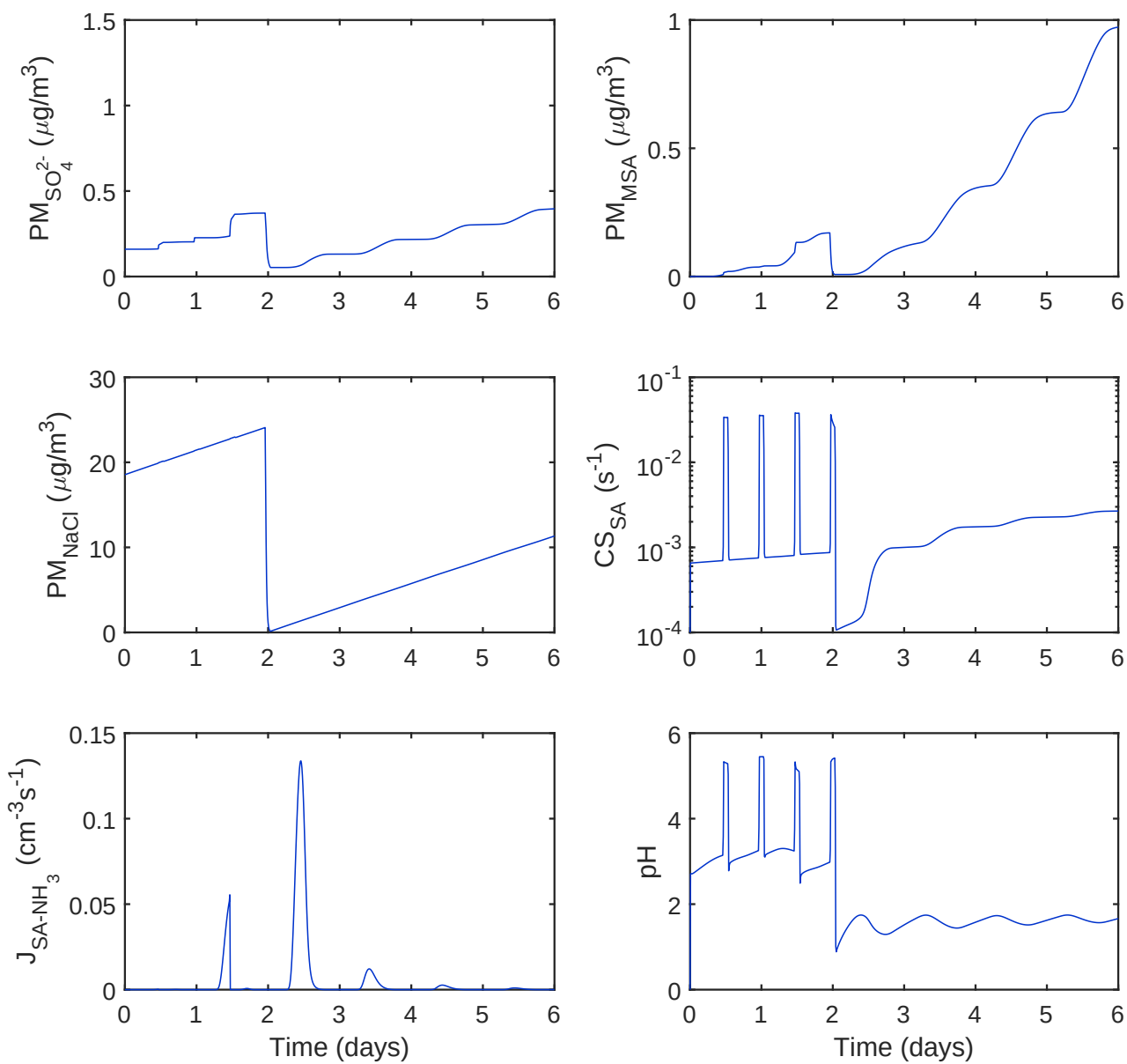


Figure S3. Total SO_4^{2-} , MSA and NaCl PM along with the SA condensation sink, SA- NH_3 driven nucleation rate and bulk pH in the BaseCase Simulation.

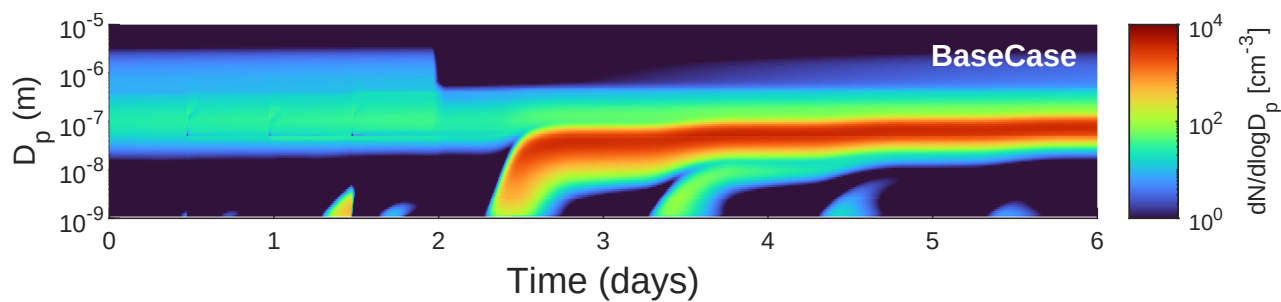


Figure S4. Aerosol particle number size distributions throughout the full simulation period in the BaseCase Simulation.

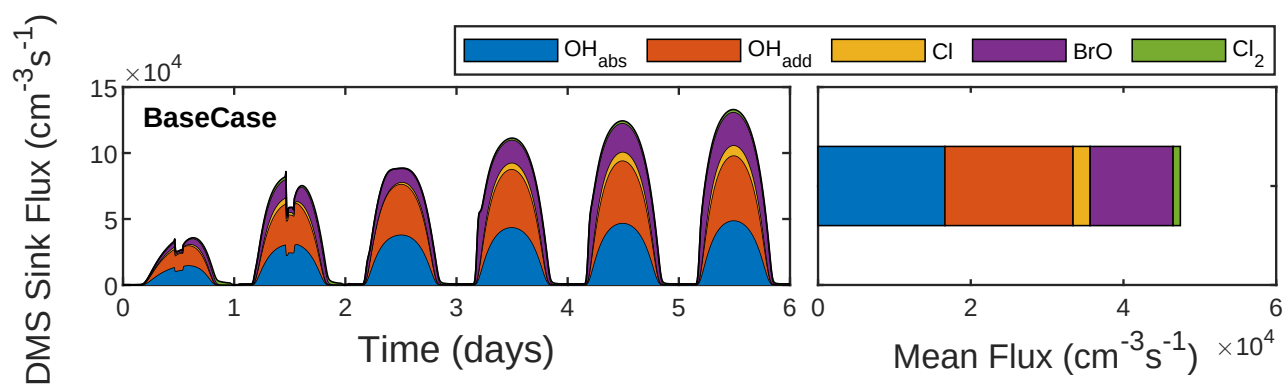


Figure S5. DMS sink flux driven by the reaction with OH (addition), OH (abstraction), Cl, BrO and Cl_2 in the BaseCase Simulation. Reactions that contribute < 1% of the total sink flux are not displayed in the figure.

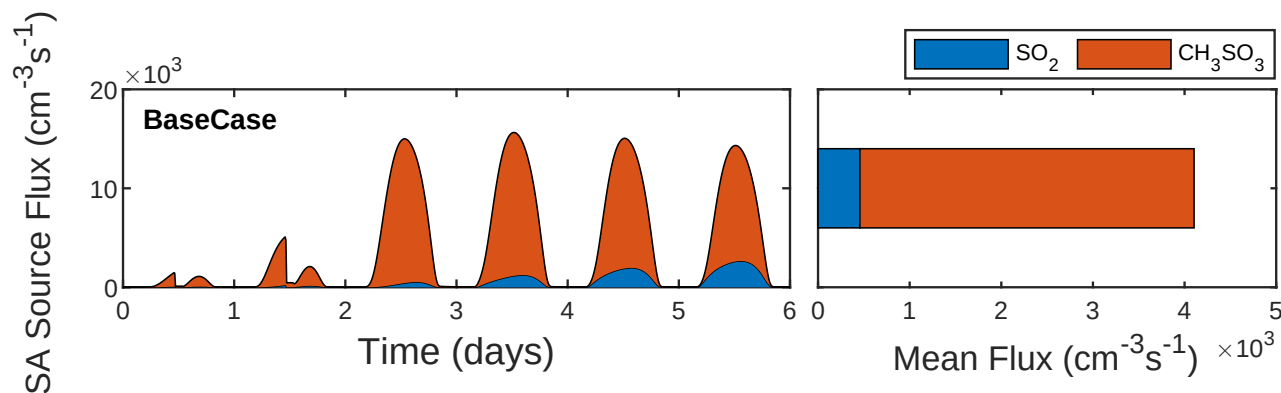


Figure S6. SA source flux from SO_2 and CH_3SO_3 in the BaseCase Simulation.

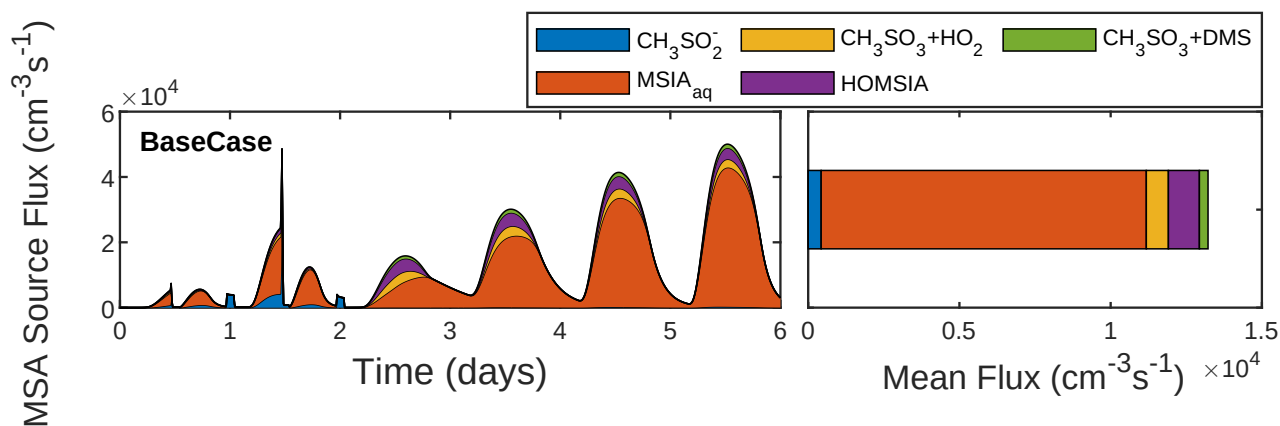


Figure S7. MSA source flux from CH_3SO_2^- and MSIA_{aq} in the aqueous-phase in addition to CH_3SO_3 via HO_2 , CH_3SO_3 via DMS and HOMSA in the gas-phase in the BaseCase Simulation.

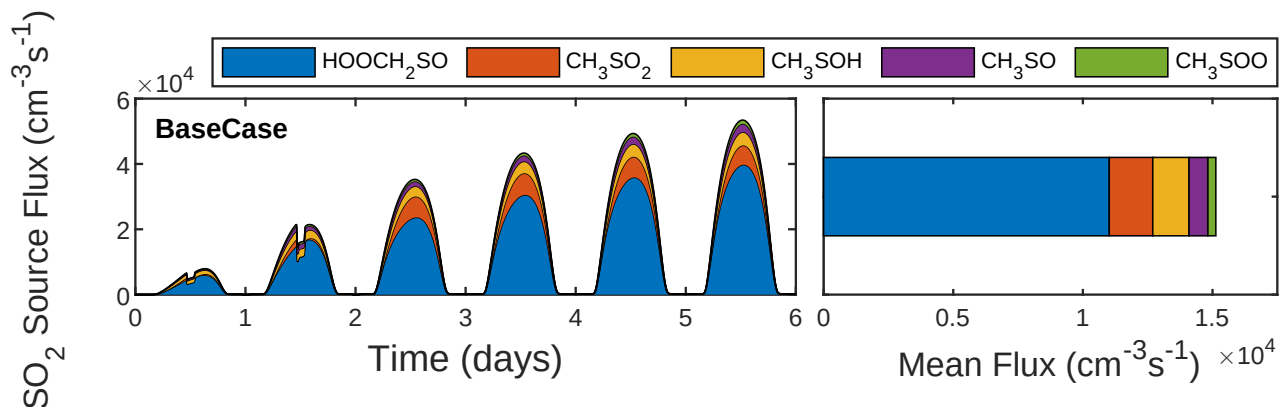


Figure S8. SO_2 source flux from HOOCH_2SO , CH_3SO_2 , CH_3SOH , CH_3SO and CH_3SOO in the BaseCase Simulation. Reactions that contribute < 1% of the total source flux are not displayed in the figure.

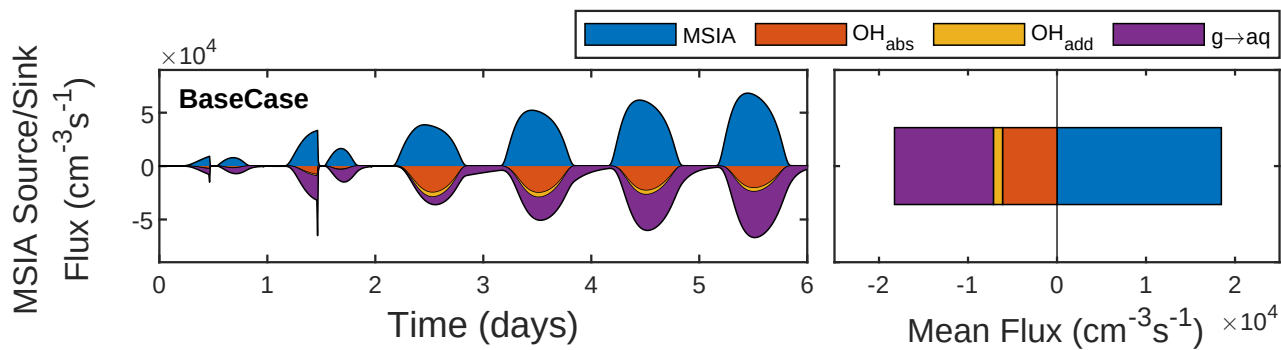


Figure S9. MSIA source/sink flux from DMSO and via reaction with OH (abstraction), OH (addition) and gas-aqueous phase uptake in the BaseCase Simulation. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

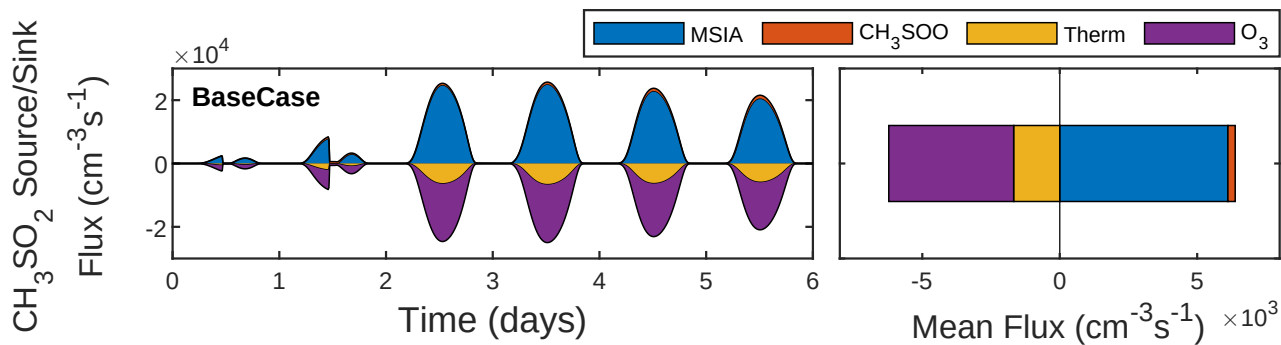


Figure S10. CH₃SO₂ source/sink flux from MSIA, CH₃SOO and via thermal decomposition and reaction with O₃ in the BaseCase Simulation. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

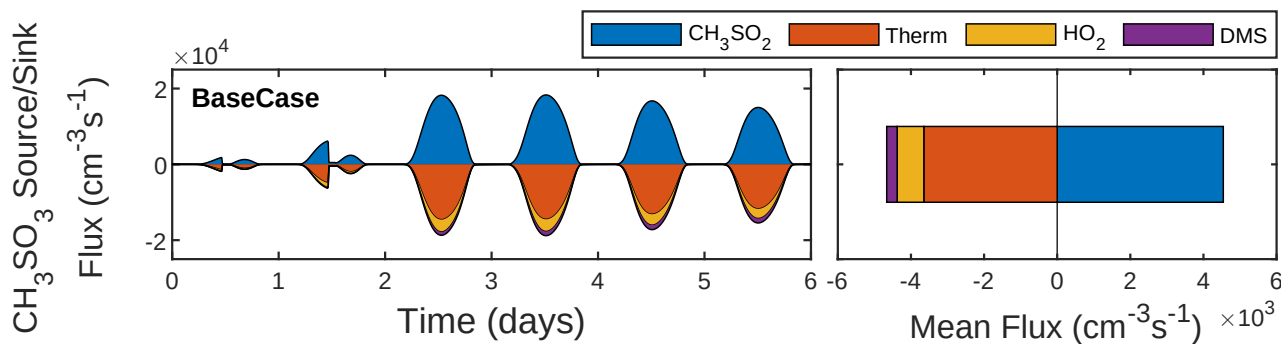


Figure S11. CH₃SO₃ source/sink flux from CH₃SO₂, via thermal decomposition and reaction with HO₂ and DMS in the BaseCase Simulation. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

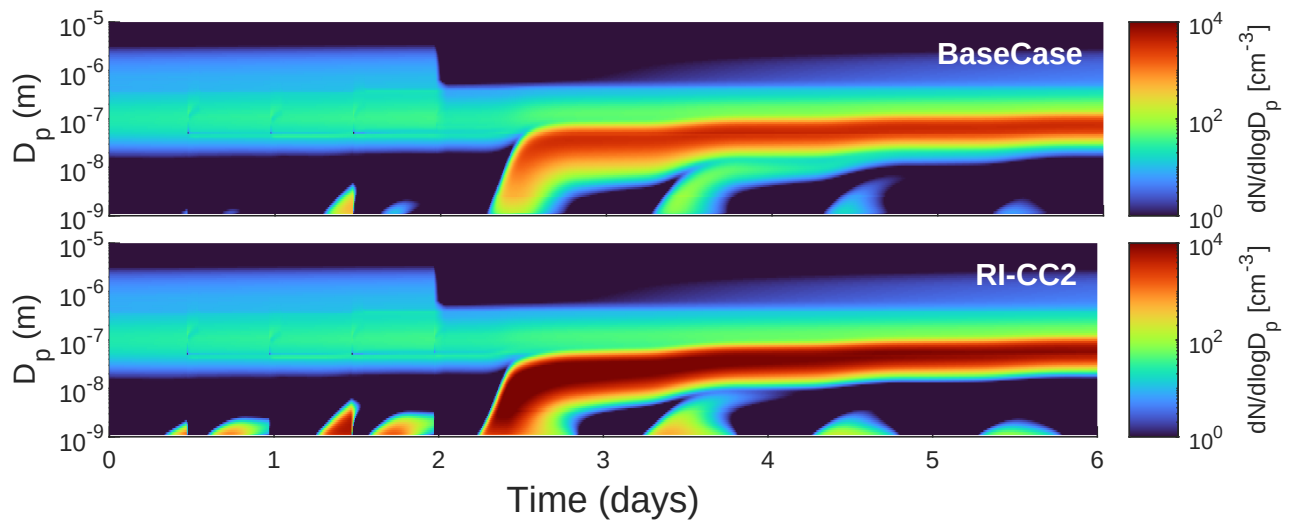


Figure S12. Aerosol particle number size distributions throughout the full simulation period in the BaseCase simulation and a sensitivity run utilizing the RI-CC2 method to calculate the nucleation rate.

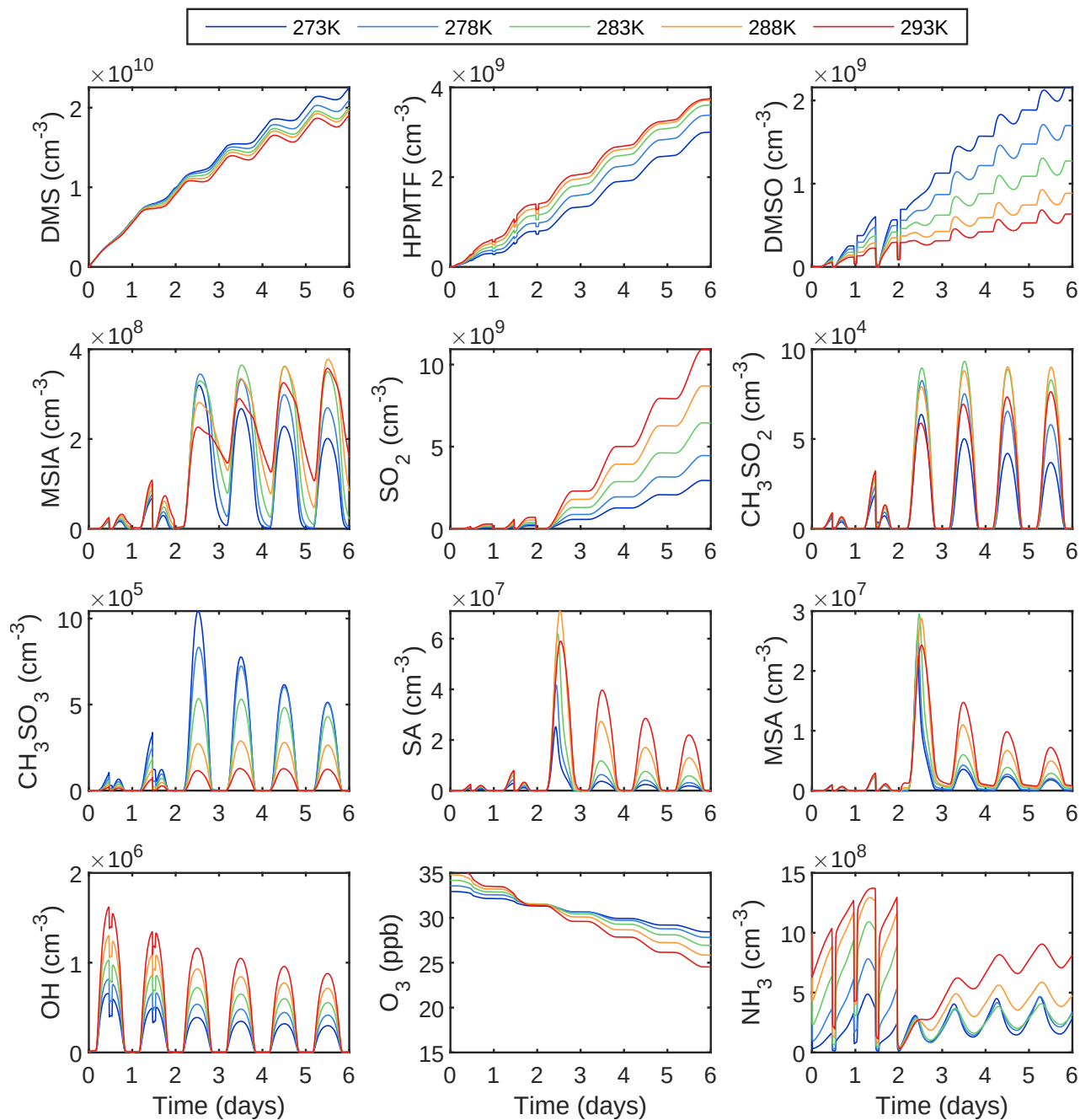


Figure S13. Concentrations of key gas-phase species at varying temperatures ranging from 273K to 293K.

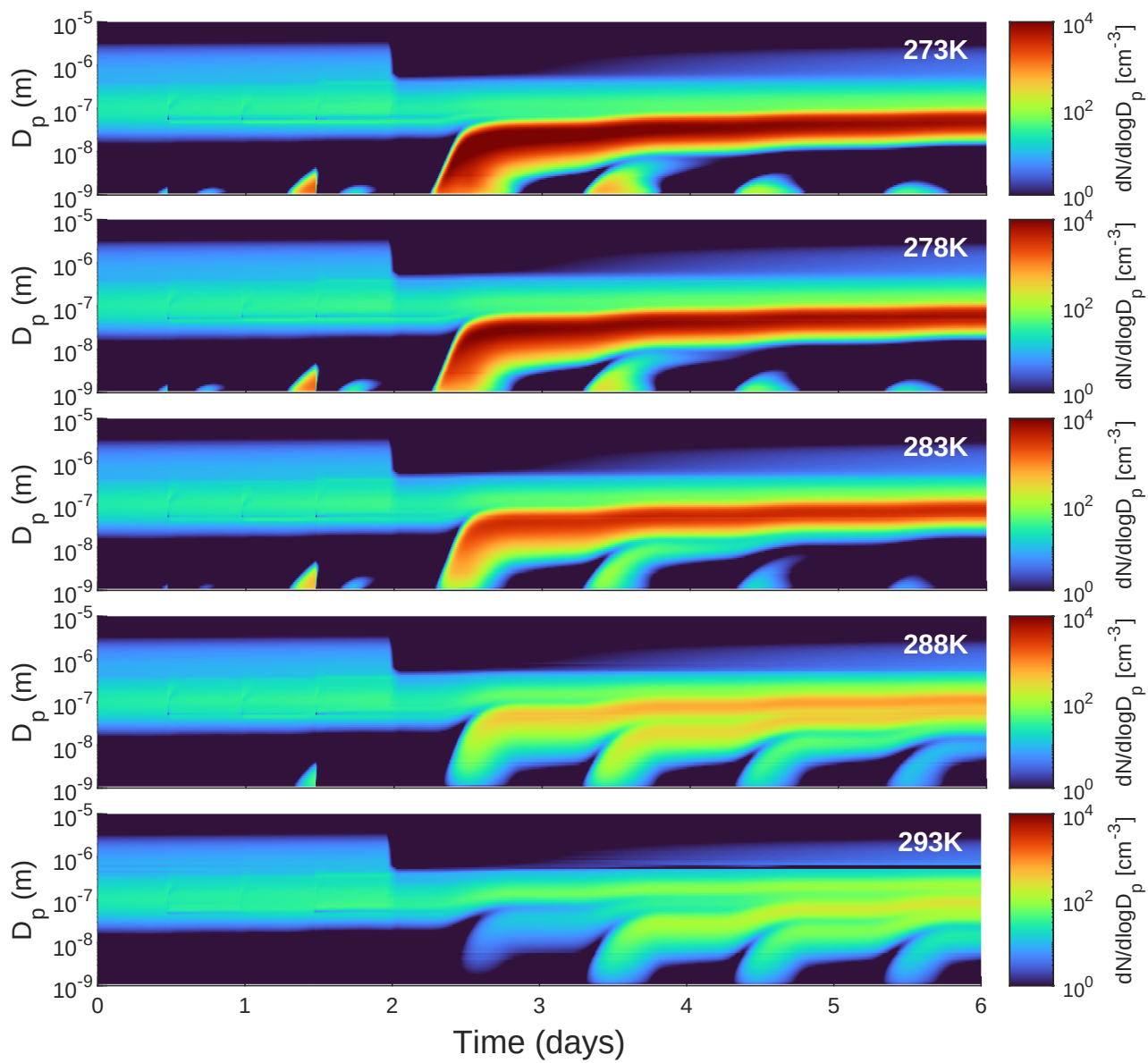


Figure S14. Aerosol particle number size distributions throughout the full simulation period at varying temperatures ranging from 273K to 293K.

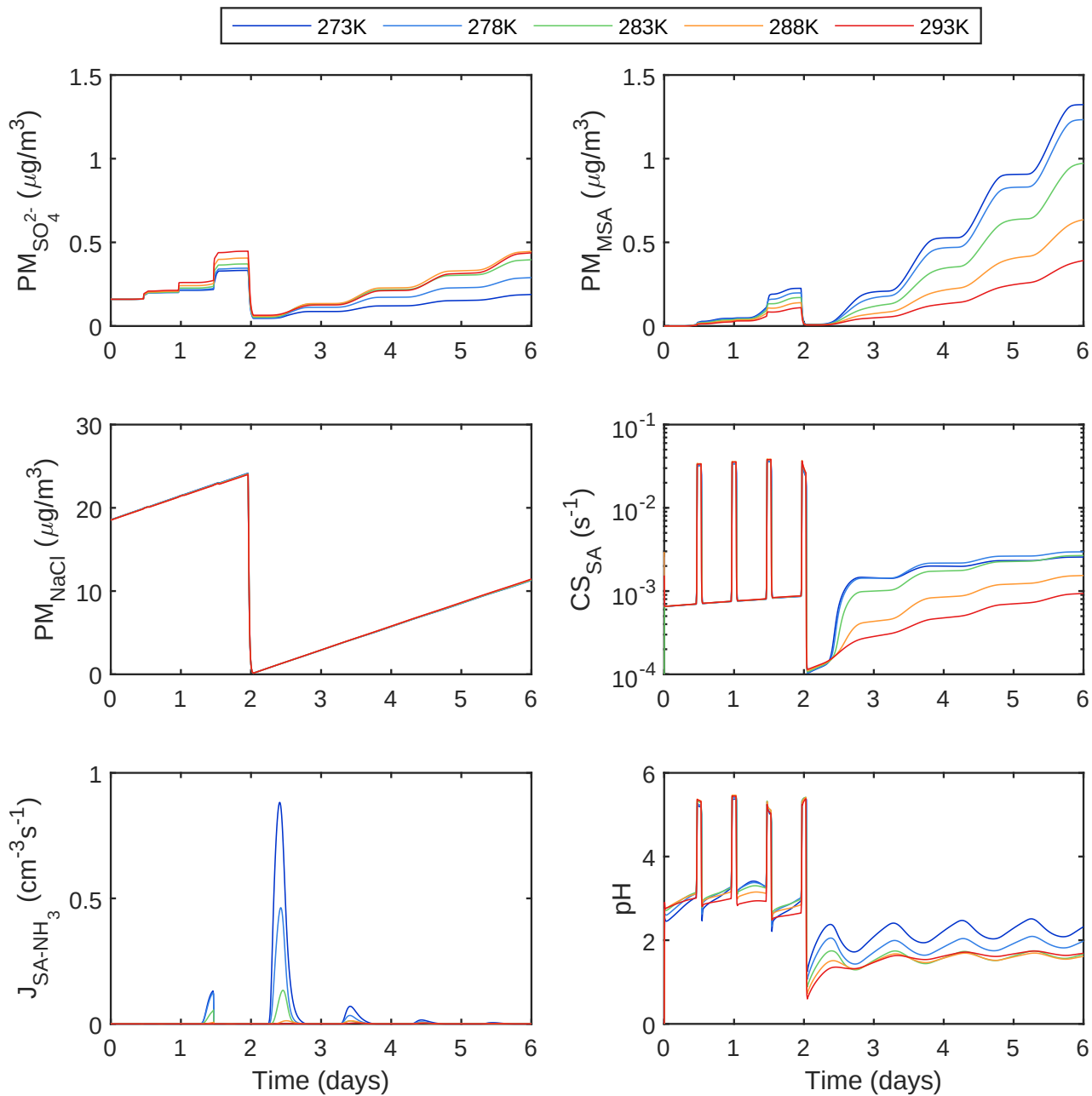


Figure S15. Total SO_4^{2-} , MSA and NaCl PM along with the SA condensation sink, SA- NH_3 driven nucleation rate and bulk pH at varying temperatures ranging from 273K to 293K.

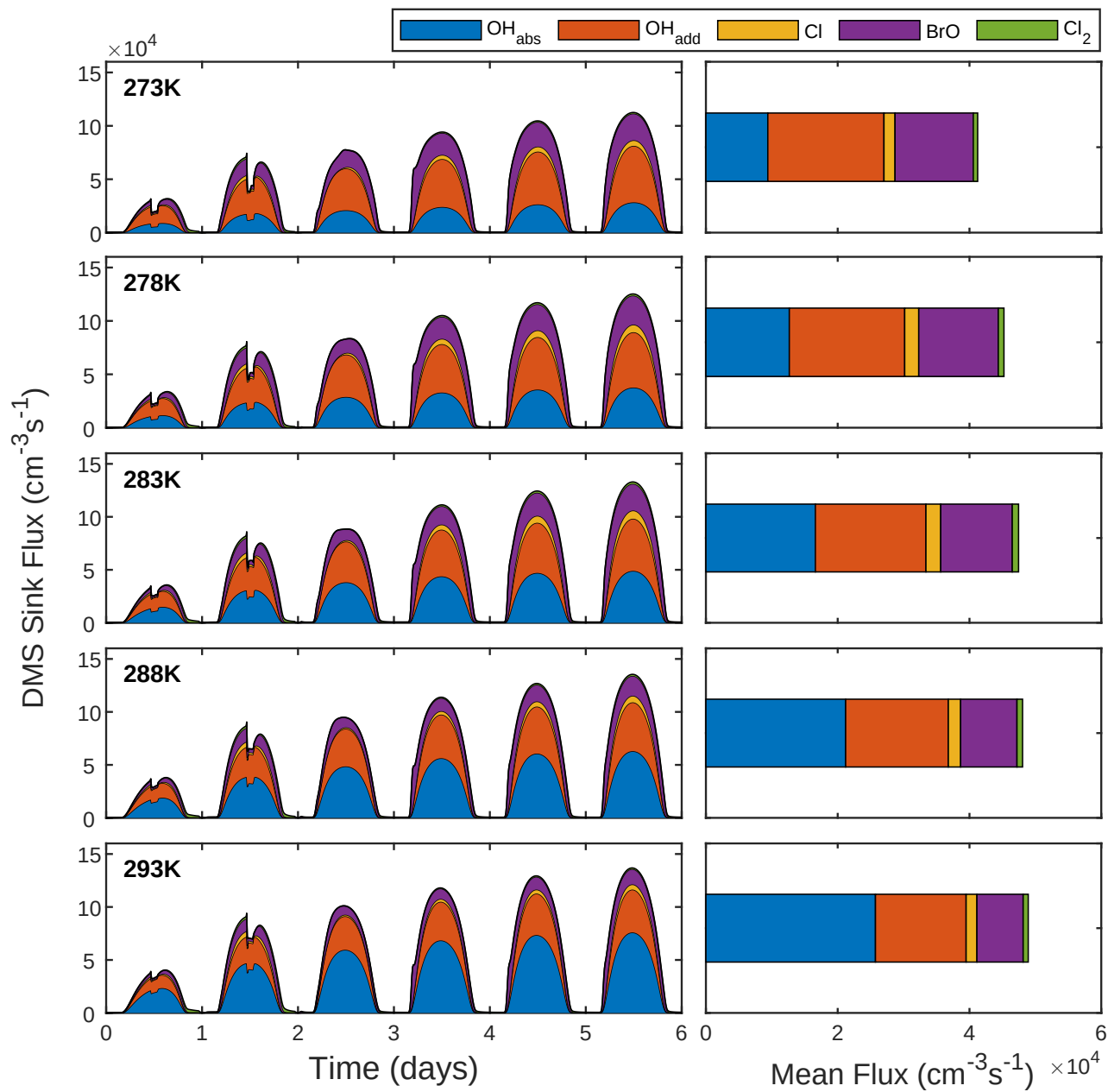


Figure S16. DMS sink flux driven by the reaction with OH (addition), OH (abstraction), Cl, BrO and Cl₂ at varying temperatures ranging from 273K to 293K. Reactions that contribute < 1% of the total sink flux are not displayed in the figure.

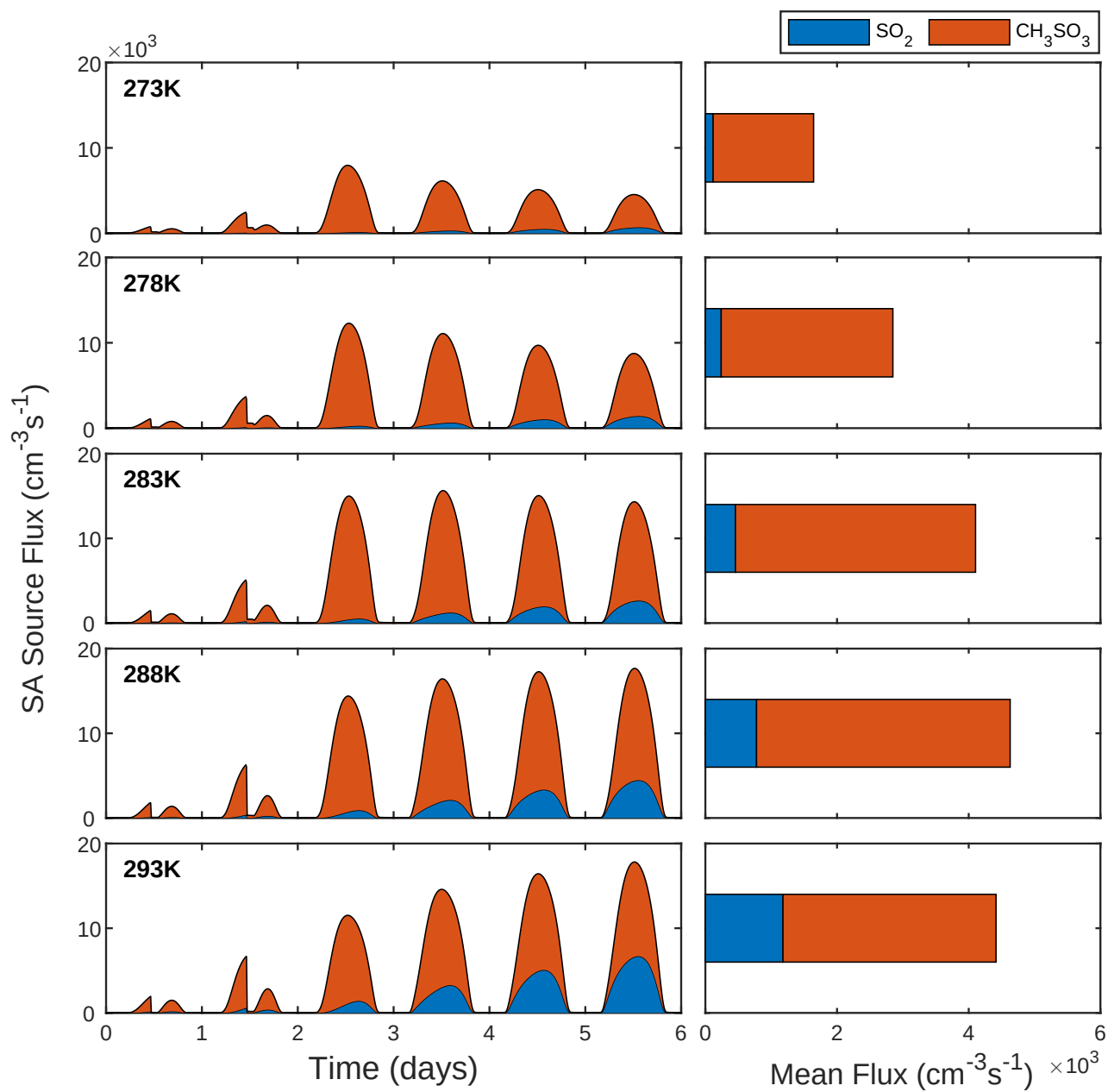


Figure S17. SA source flux from SO_2 and CH_3SO_3 at varying temperatures ranging from 273K to 293K.

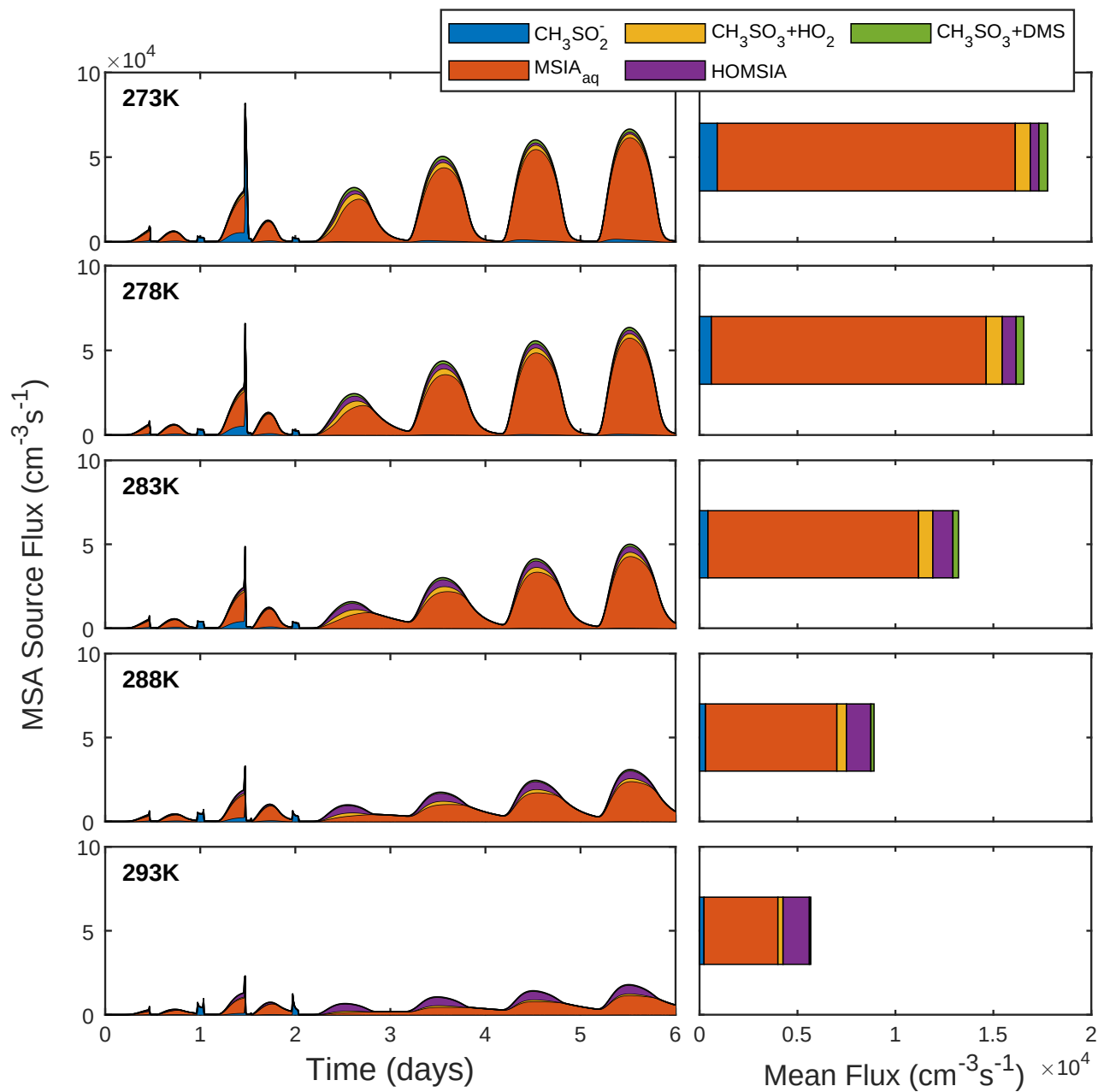


Figure S18. MSA source flux from CH_3SO_2^- and MSIA_{aq} in the aqueous-phase in addition to CH_3SO_3 via HO_2 , CH_3SO_3 via DMS and HOMSIA in the gas-phase at varying temperatures ranging from 273K to 293K.

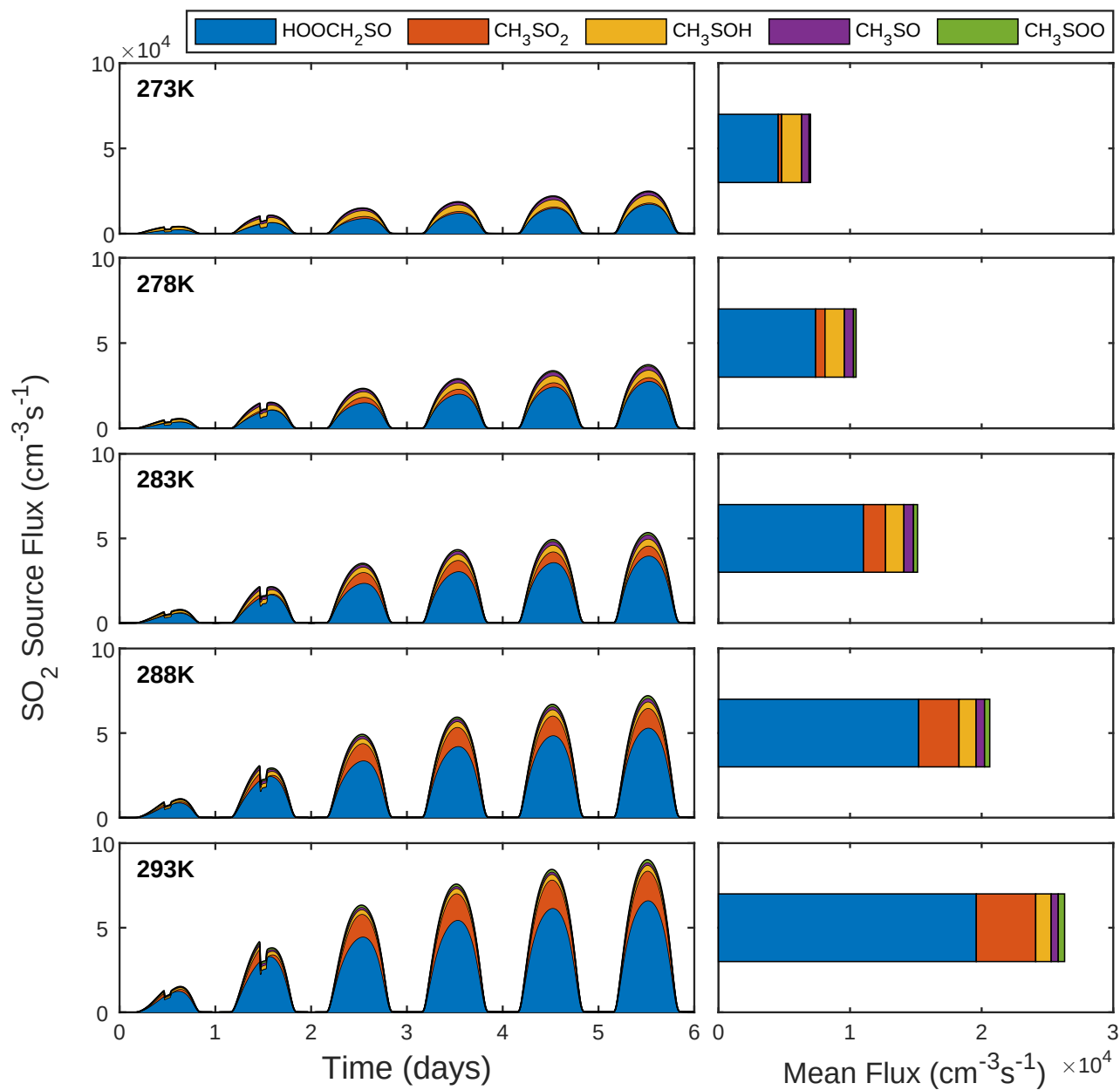


Figure S19. SO₂ source flux from HOOCH₂SO, CH₃SO₂, CH₃SOH, CH₃SO and CH₃SOO at varying temperatures ranging from 273K to 293K. Reactions that contribute < 1% of the total source flux are not displayed in the figure.

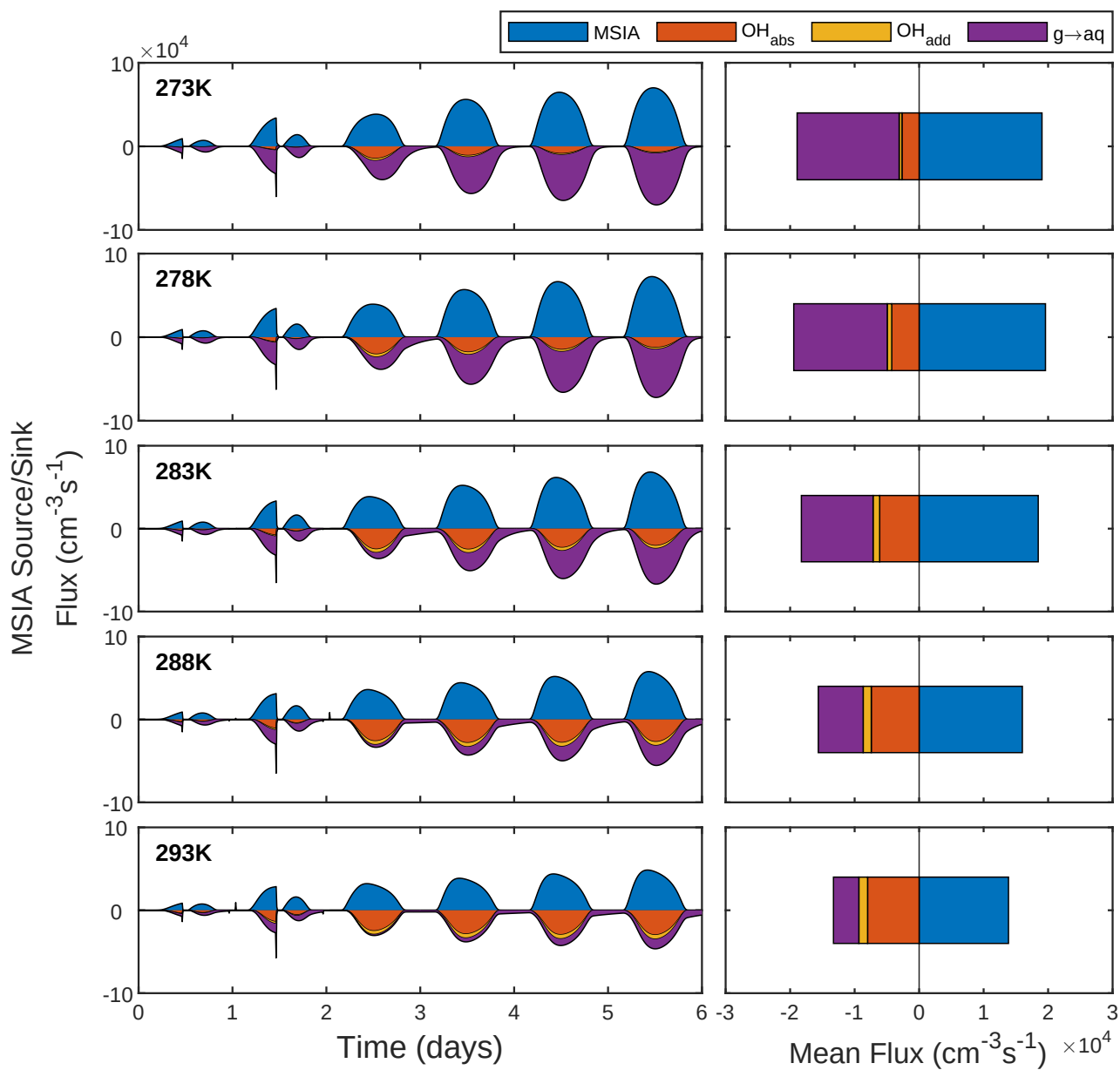


Figure S20. MSIA source/sink flux from DMSO and via reaction with OH (abstraction), OH (addition) and gas-aqueous phase uptake at varying temperatures ranging from 273K to 293K. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

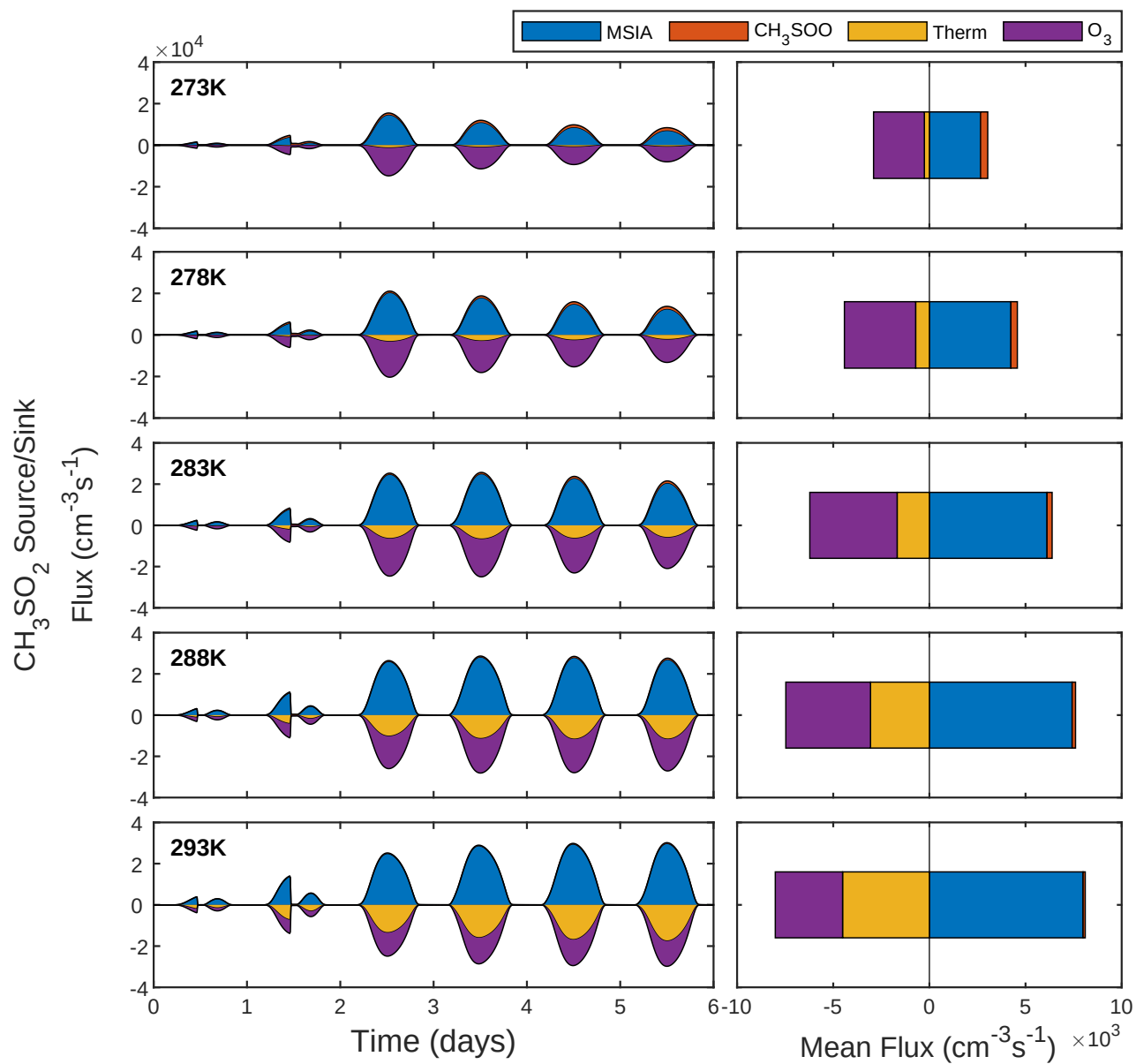


Figure S21. CH_3SO_2 source/sink flux from MSIA, CH_3SOO and via thermal decomposition and reaction with O_3 at varying temperatures ranging from 273K to 293K. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

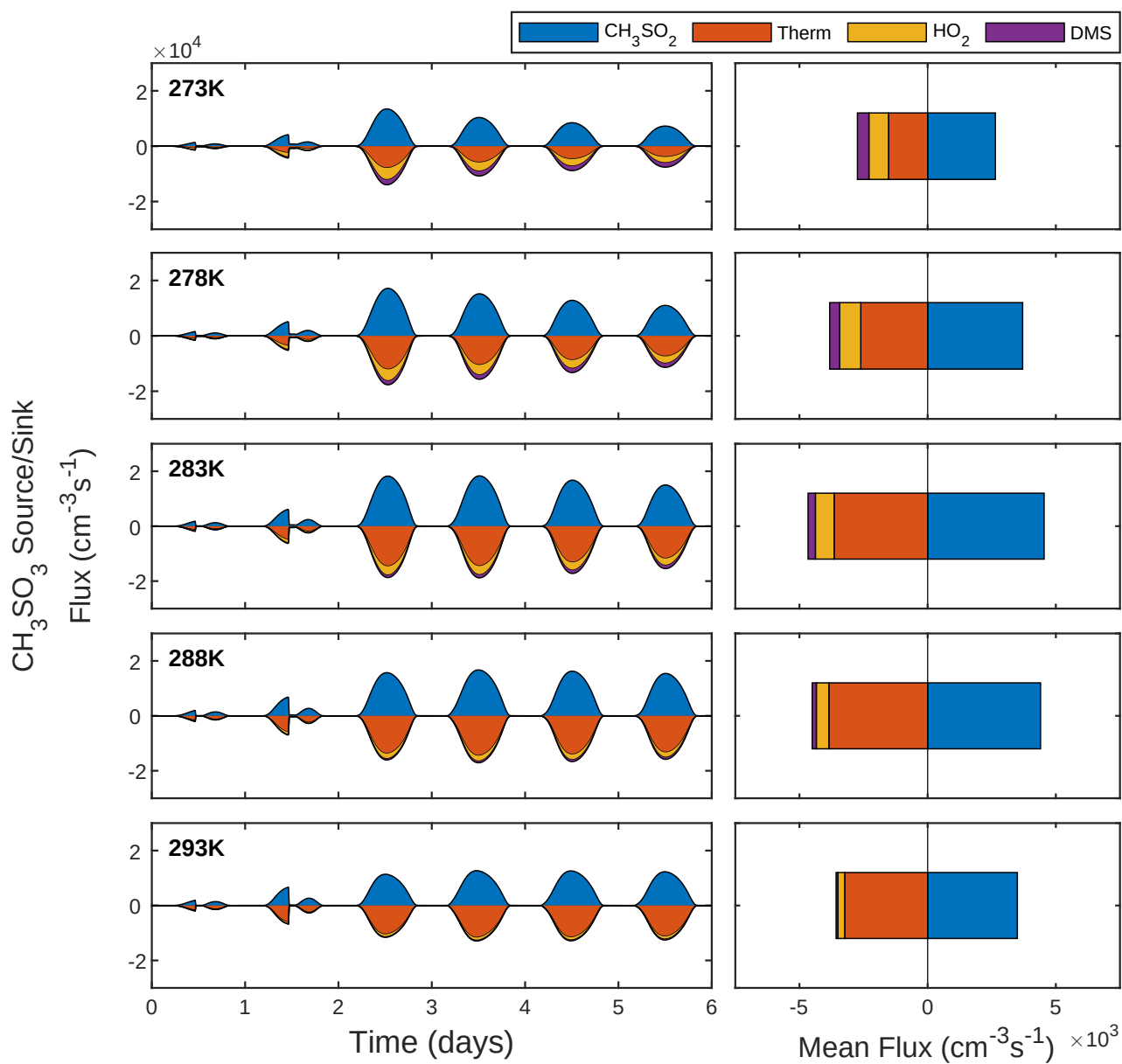


Figure S22. CH_3SO_3 source/sink flux from CH_3SO_2 , via thermal decomposition and reaction with HO_2 and DMS at varying temperatures ranging from 273K to 293K. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

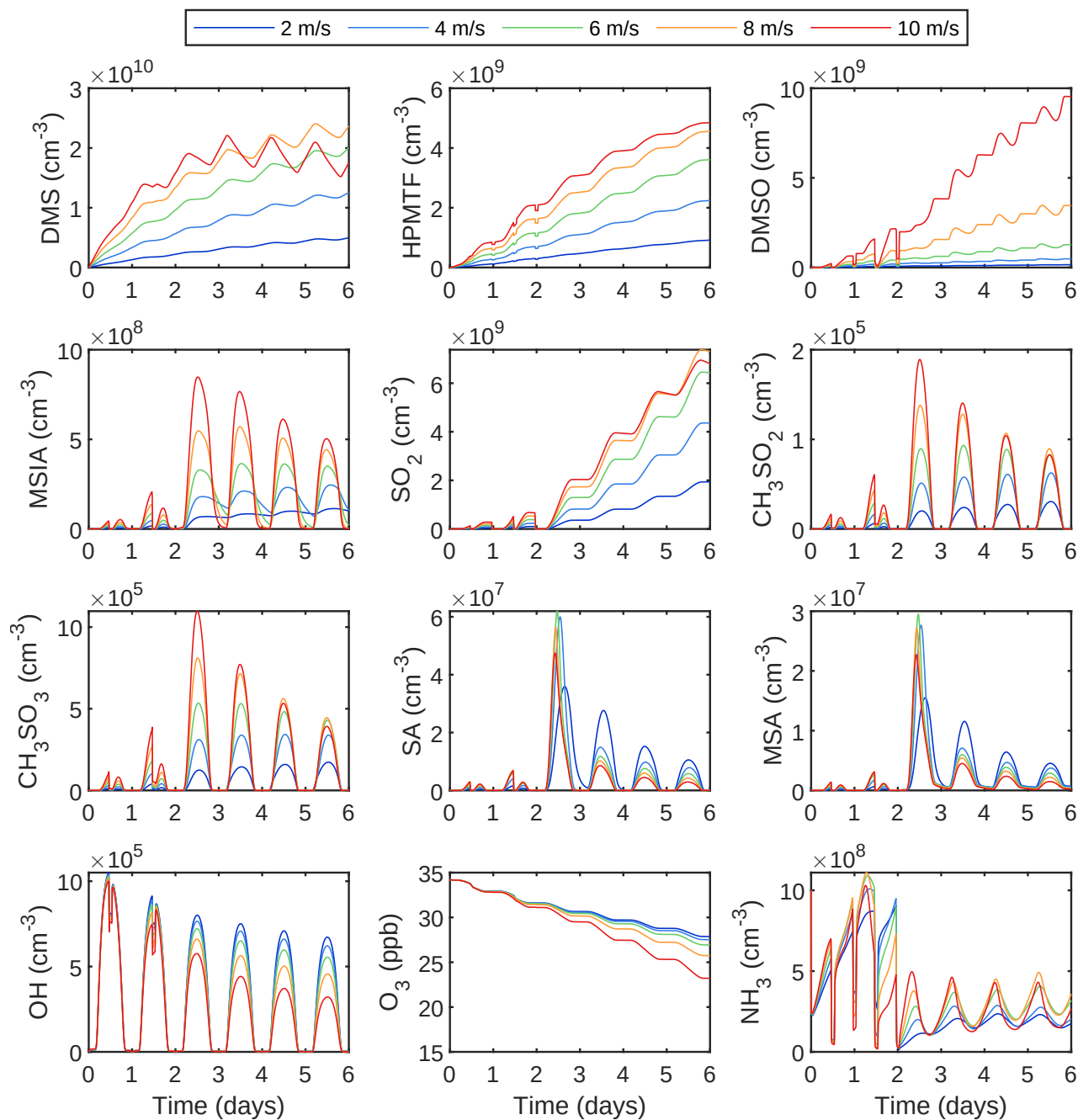


Figure S23. Concentrations of key gas-phase species at varying wind-speeds ranging from 2 m/s to 10 m/s.

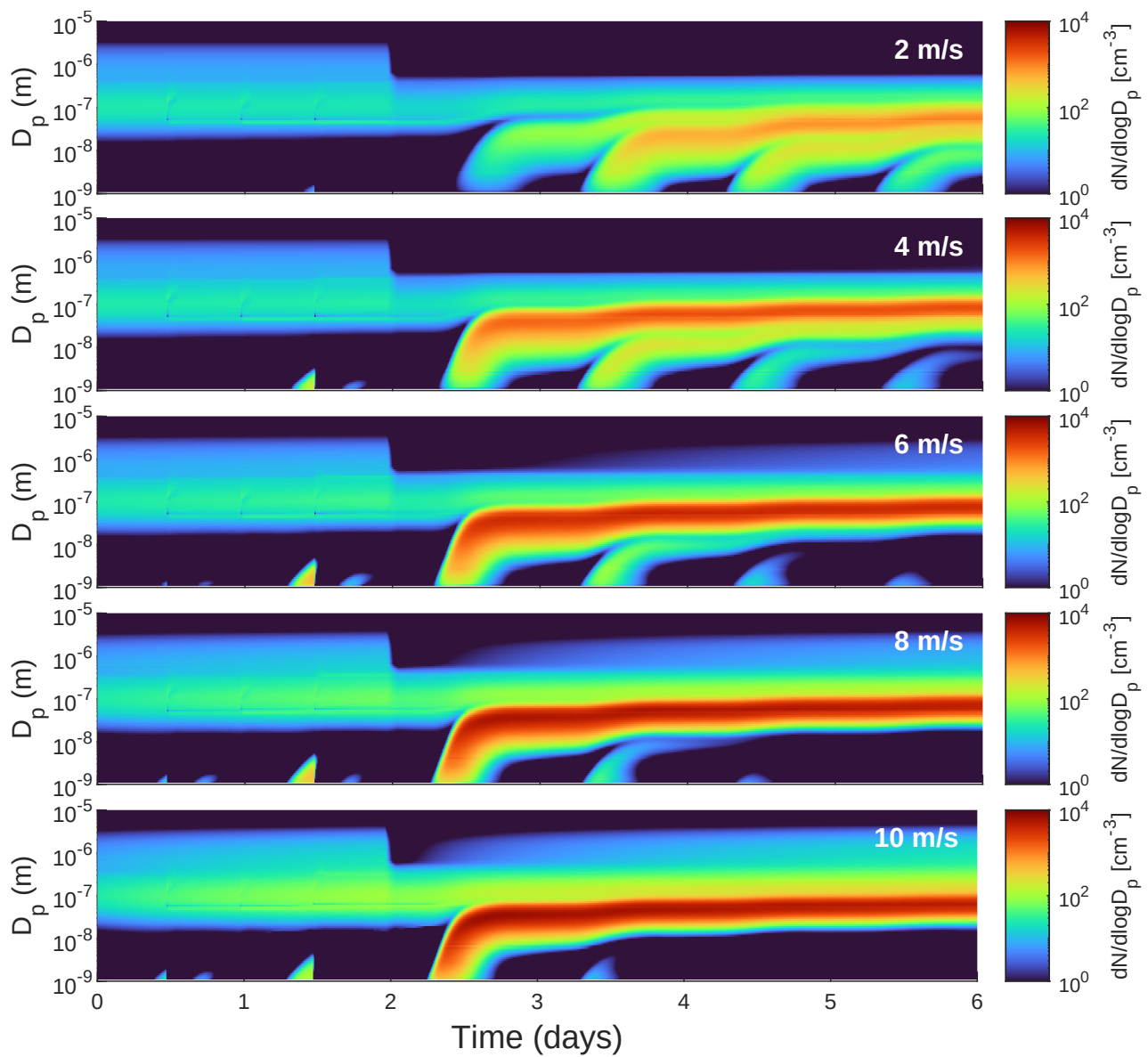


Figure S24. Aerosol particle number size distributions throughout the full simulation period at varying wind-speeds ranging from 2 m/s to 10 m/s.

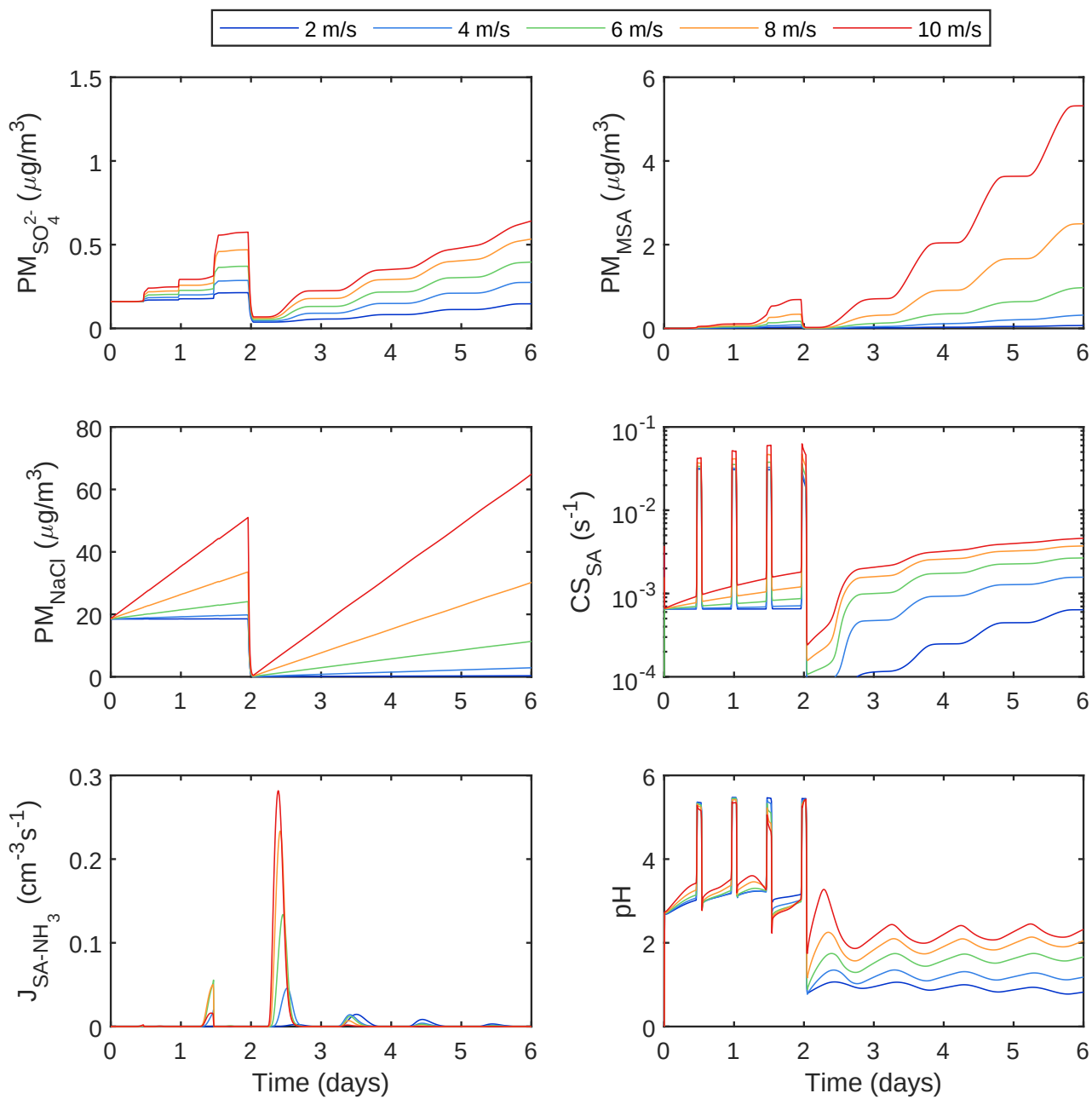


Figure S25. Total SO_4^{2-} , MSA and NaCl PM along with the SA condensation sink, SA-NH₃ driven nucleation rate and bulk pH at varying wind-speeds ranging from 2 m/s to 10 m/s.

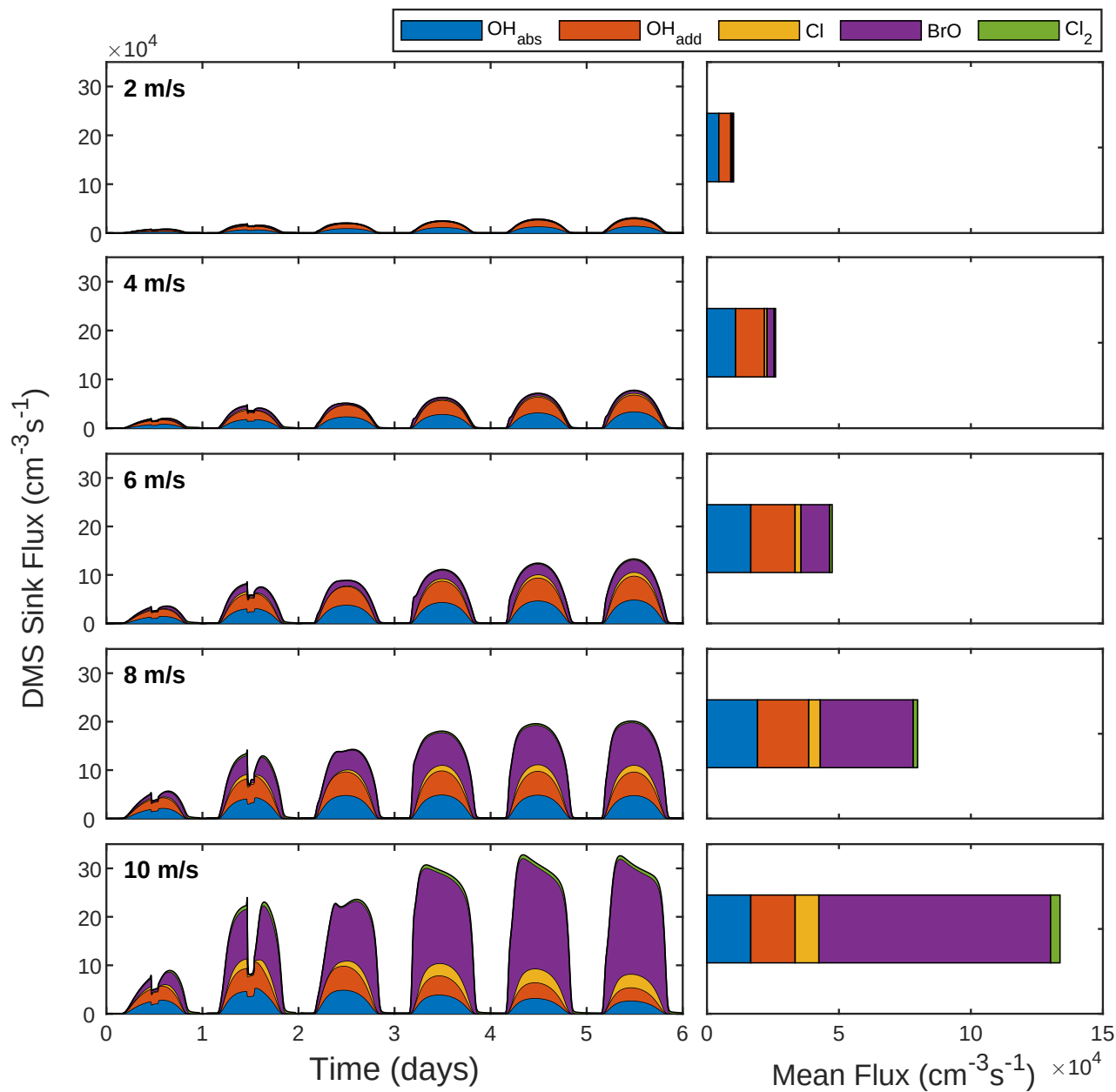


Figure S26. DMS sink flux driven by the reaction with OH (addition), OH (abstraction), Cl, BrO and Cl₂ at varying wind-speeds ranging from 2 m/s to 10 m/s. Reactions that contribute < 1% of the total sink flux are not displayed in the figure.

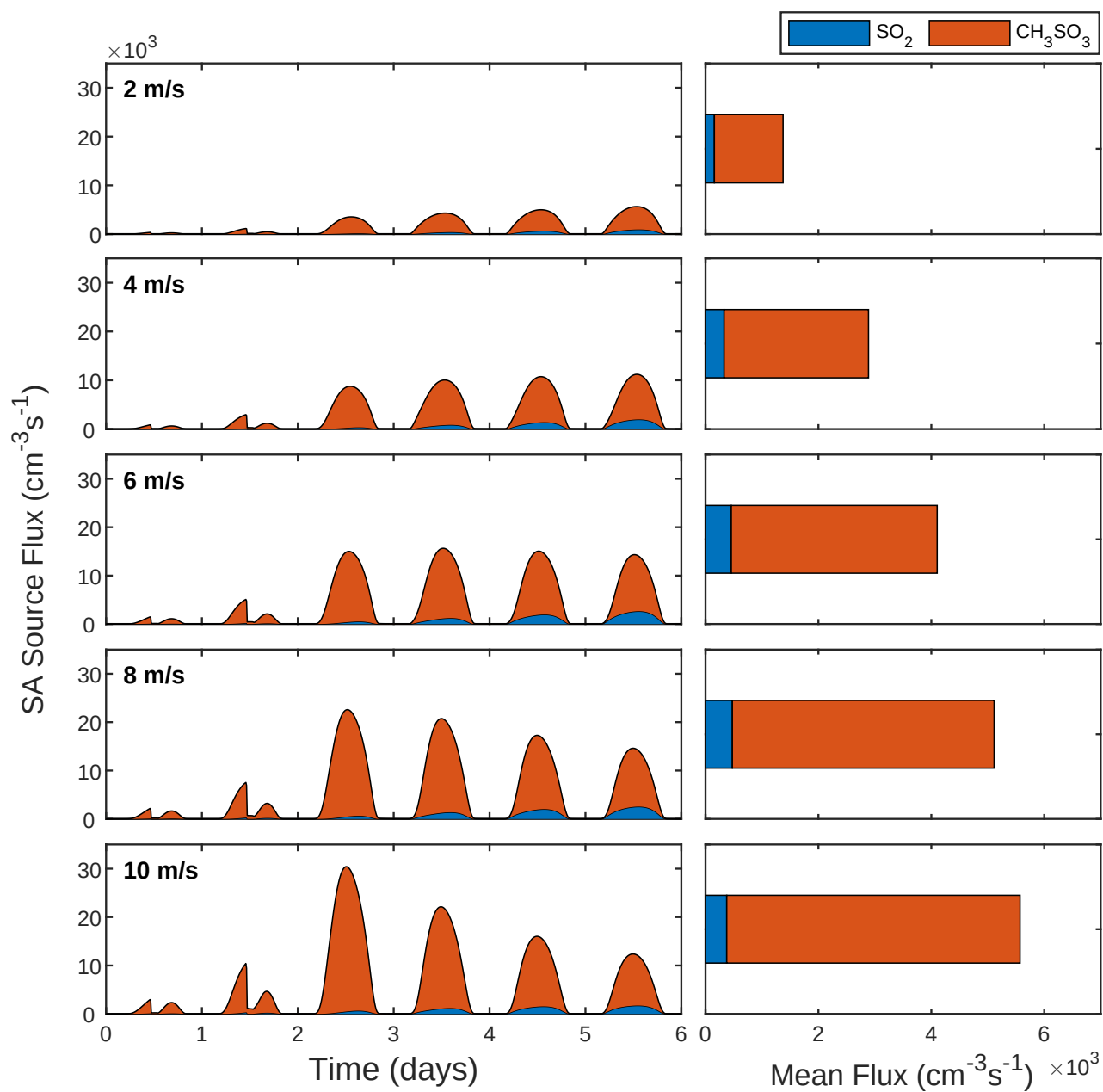


Figure S27. SA source flux from SO_2 and CH_3SO_3 at varying wind-speeds ranging from 2 m/s to 10 m/s.

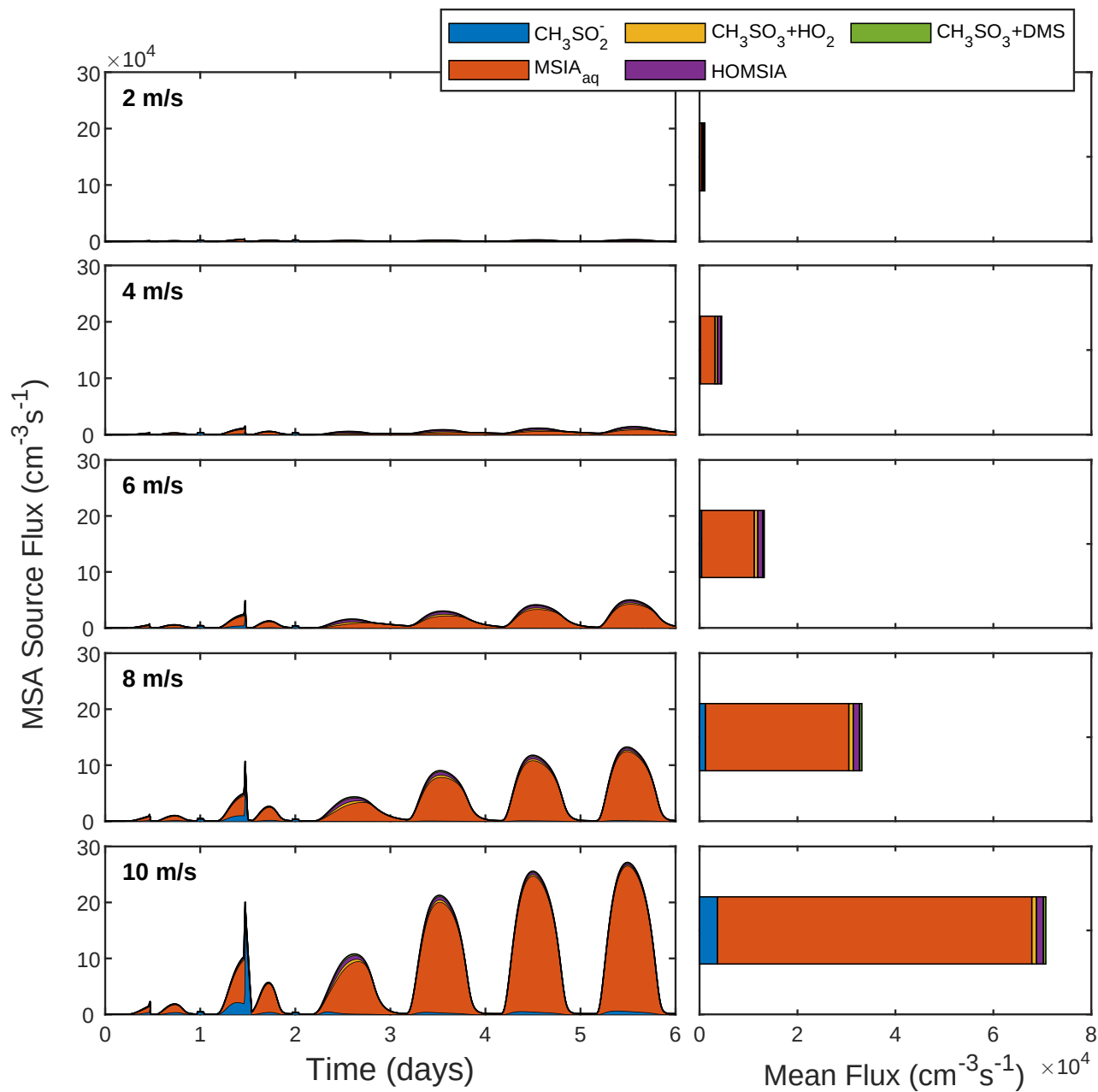


Figure S28. MSA source flux from CH_3SO_2^- and MSIA_{aq} in the aqueous-phase in addition to CH_3SO_3 via HO_2 , CH_3SO_3 via DMS and HOMSA in the gas-phase at varying wind-speeds ranging from 2 m/s to 10 m/s.

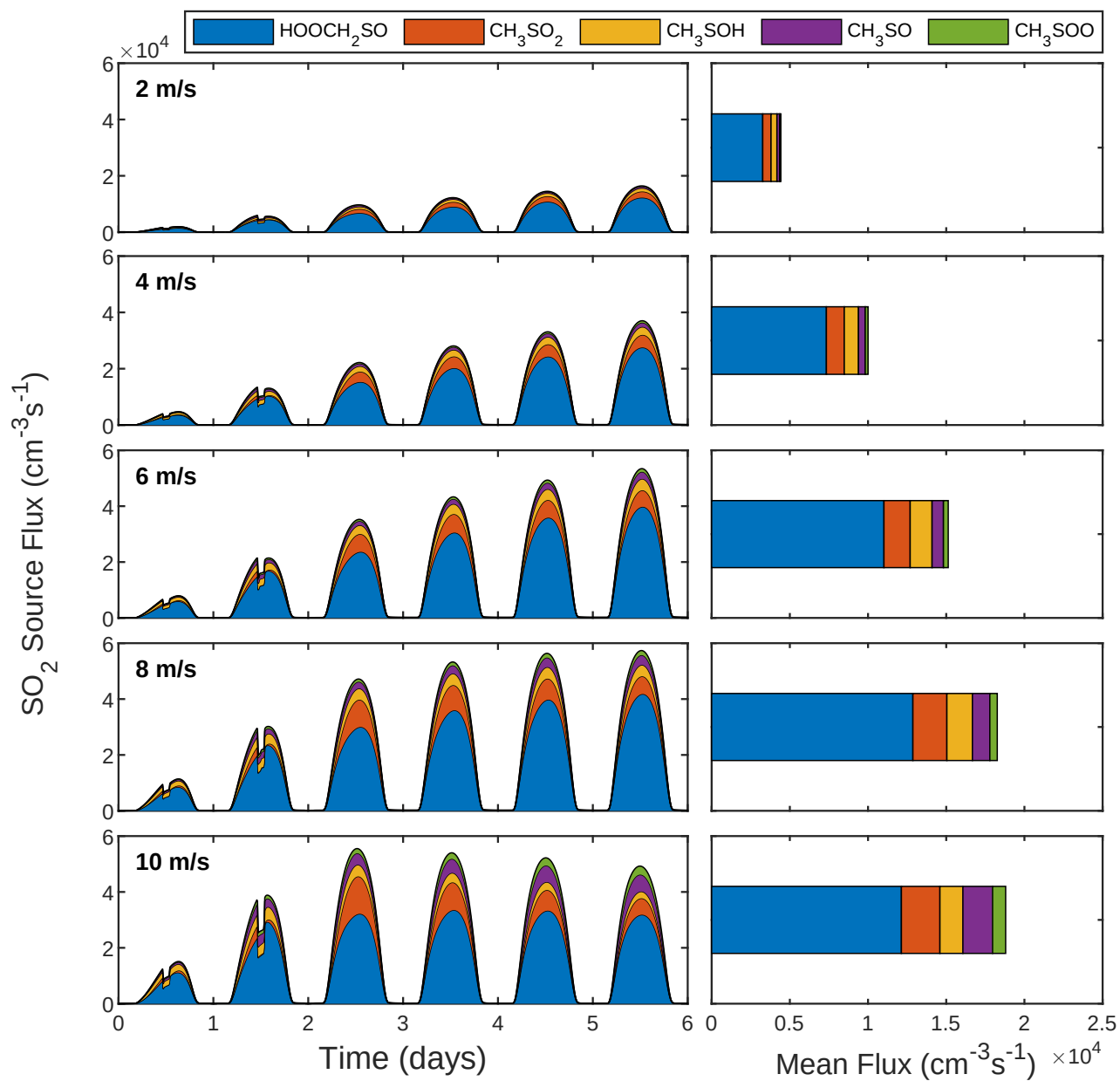


Figure S29. SO₂ source flux from HOOCH₂SO, CH₃SO₂, CH₃SOH, CH₃SO and CH₃SOO at varying wind-speeds ranging from 2 m/s to 10 m/s. Reactions that contribute < 1% of the total source flux are not displayed in the figure.

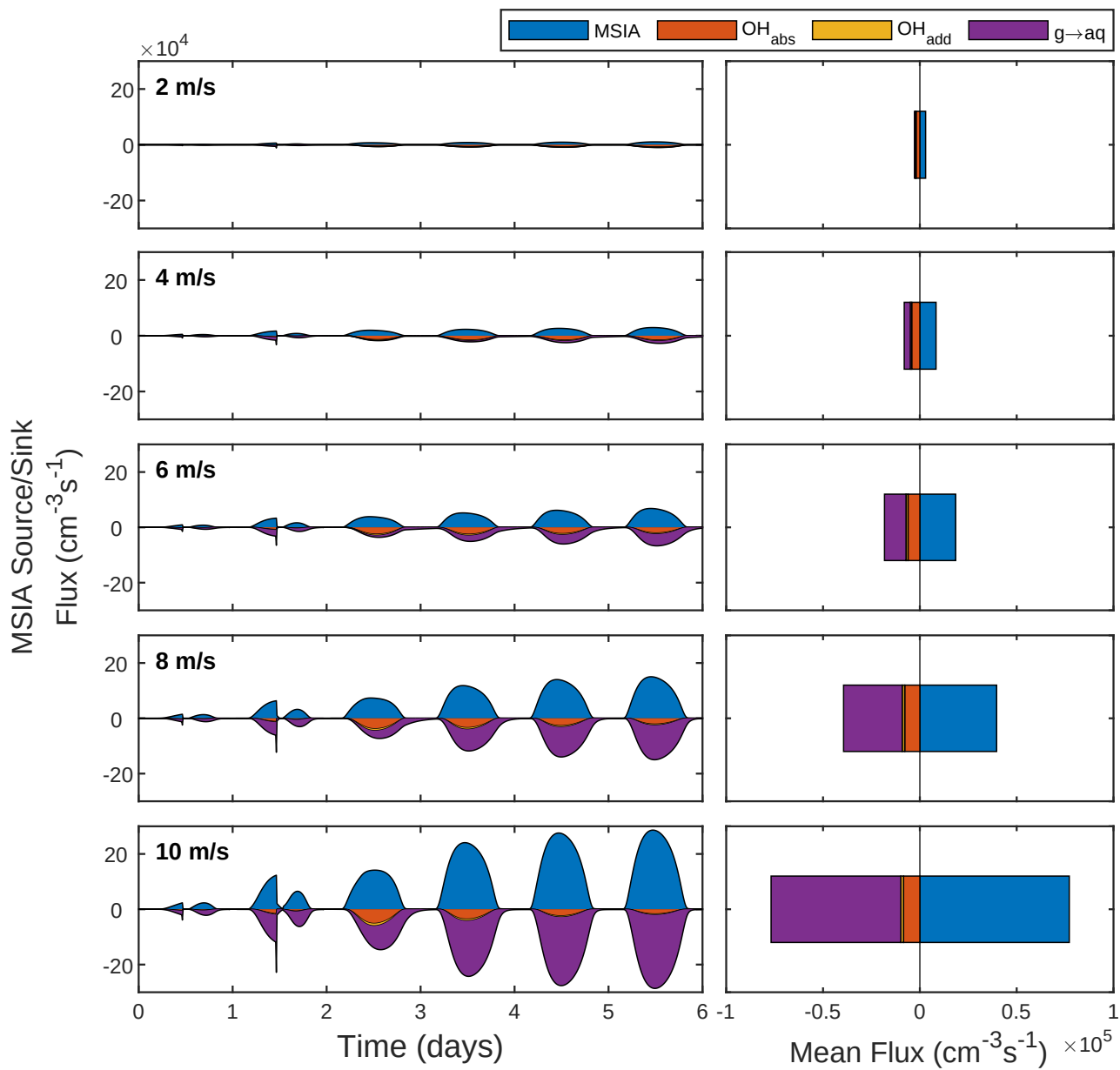


Figure S30. MSIA source/sink flux from DMSO and via reaction with OH (abstraction), OH (addition) and gas-aqueous phase uptake at varying wind-speeds ranging from 2 m/s to 10 m/s. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

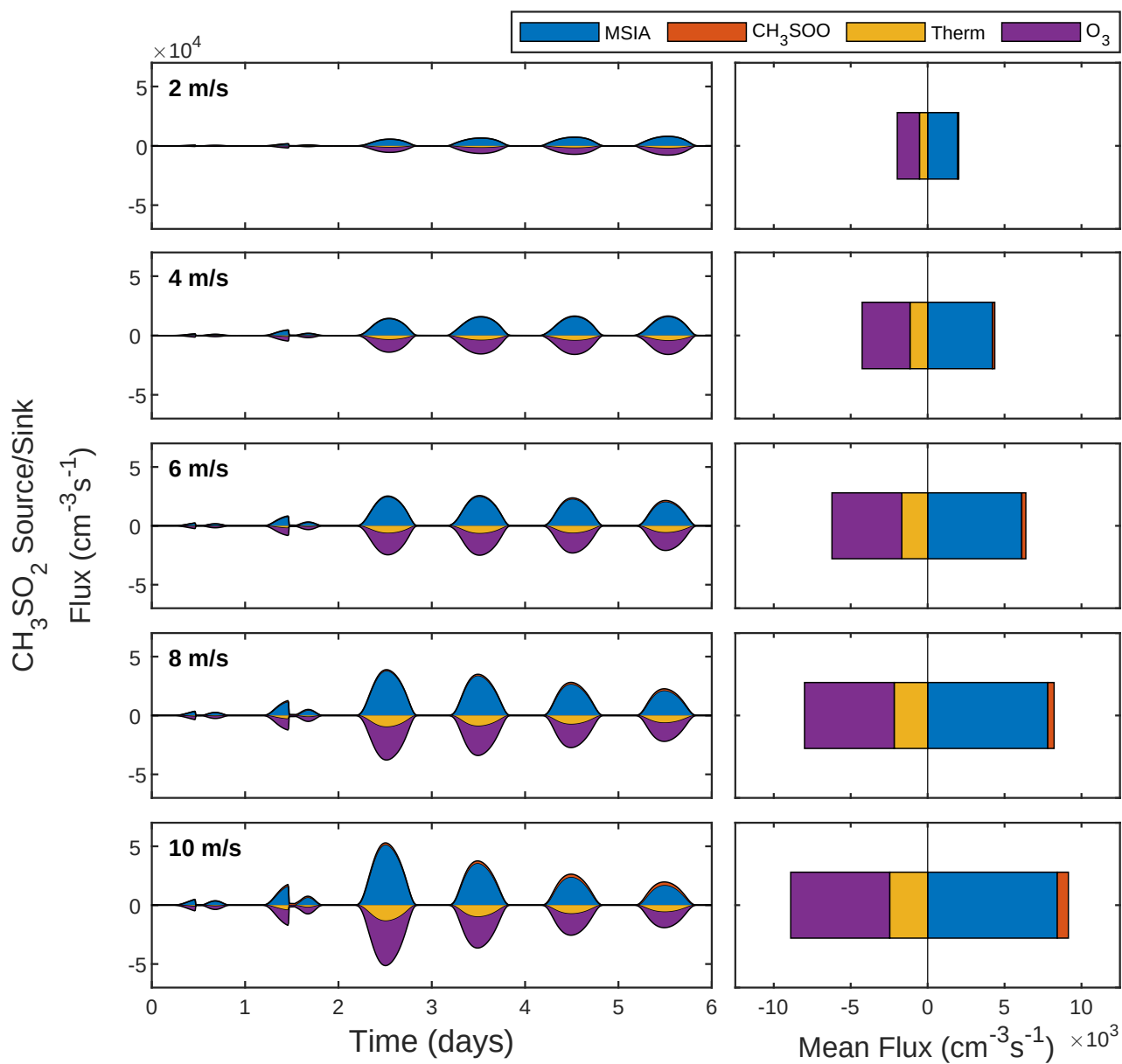


Figure S31. CH_3SO_2 source/sink flux from MSIA, CH_3SOO and via thermal decomposition and reaction with O_3 at varying wind-speeds ranging from 2 m/s to 10 m/s. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

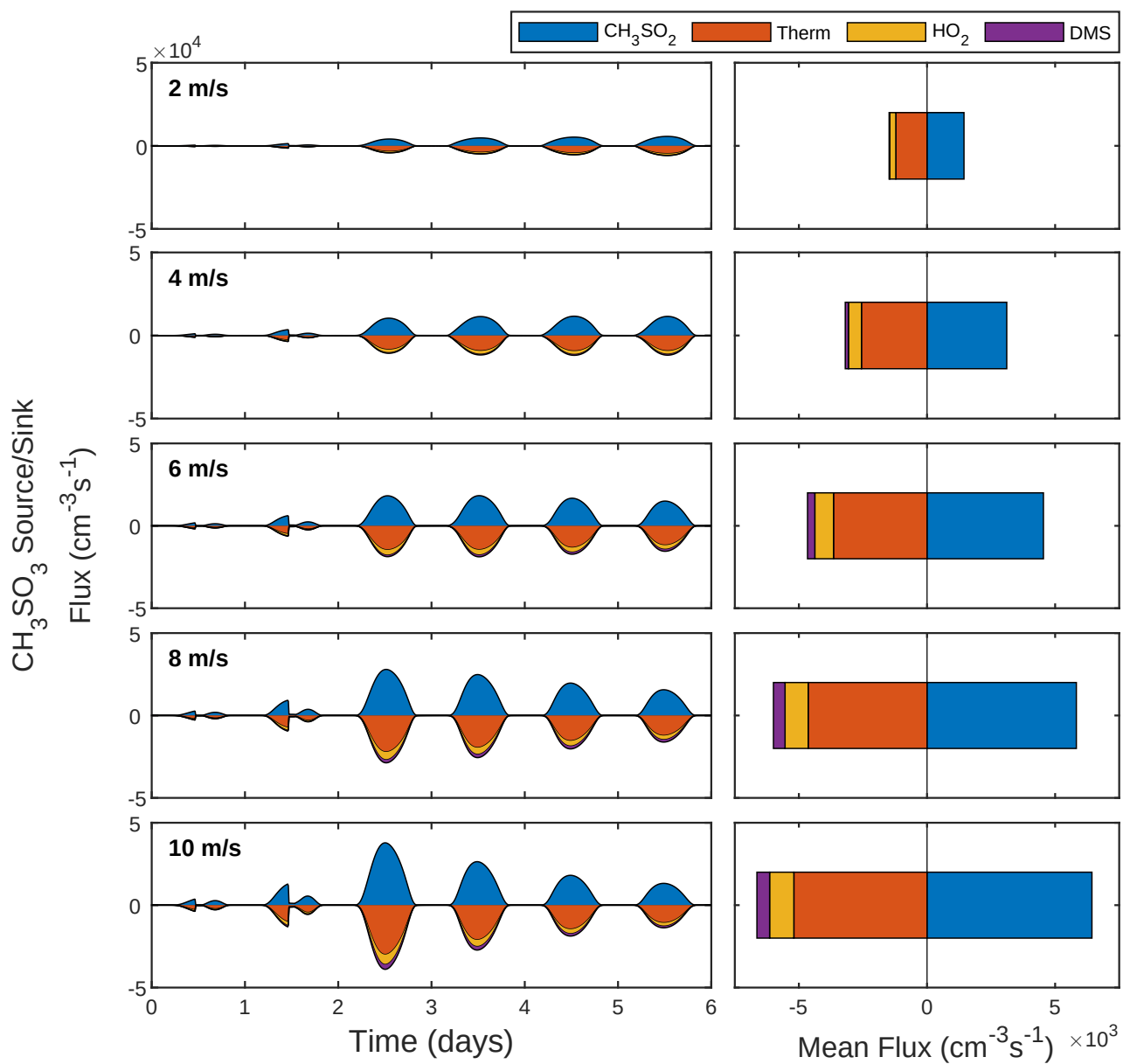


Figure S32. CH_3SO_3 source/sink flux from CH_3SO_2 , via thermal decomposition and reaction with HO_2 and DMS at varying wind-speeds ranging from 2 m/s to 10 m/s. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

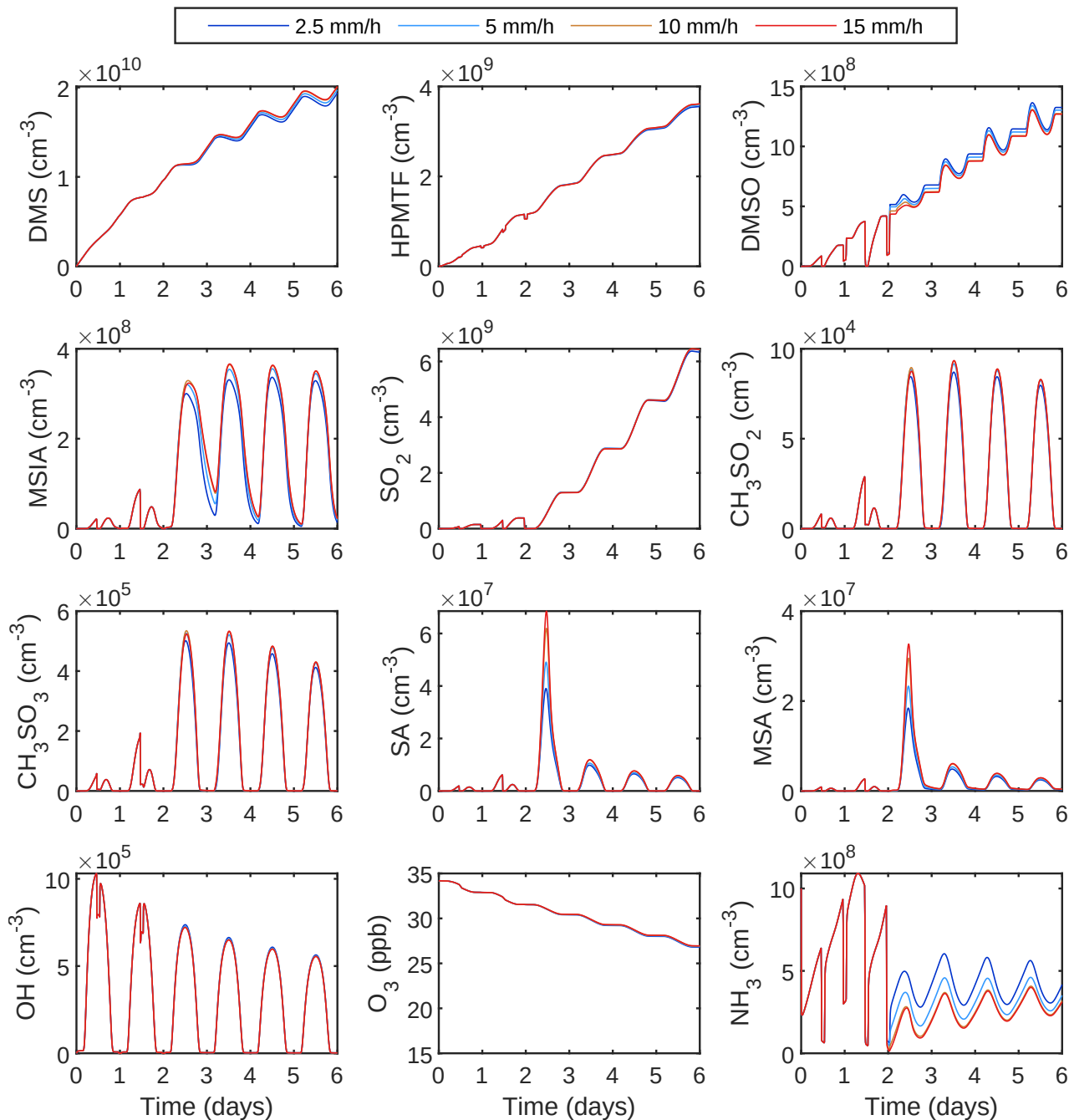


Figure S33. Concentrations of key gas-phase species at varying rates of precipitation ranging from 2.5 mm/h to 15 mm/h.

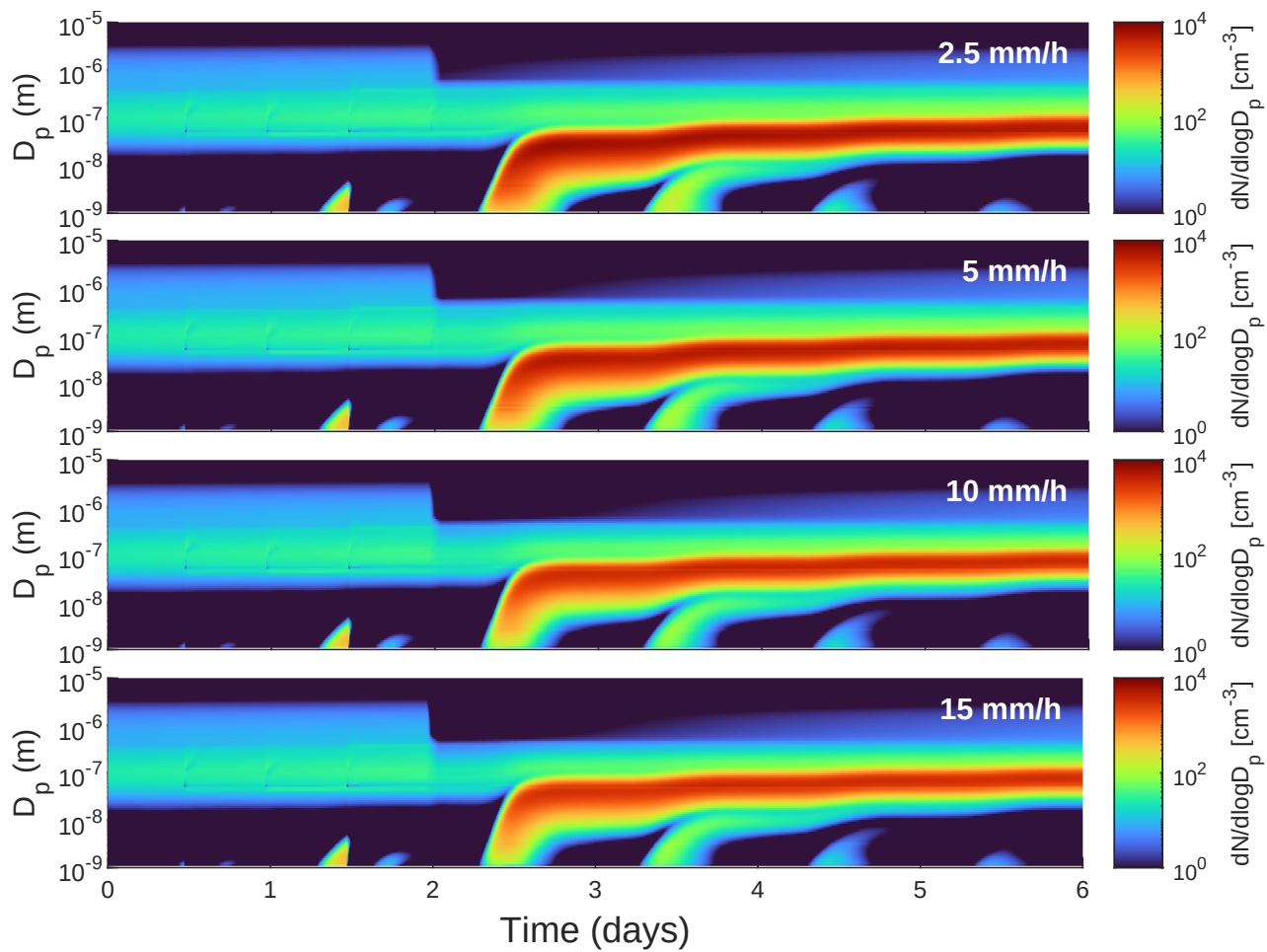


Figure S34. Aerosol particle number size distributions throughout the full simulation period at varying rates of precipitation ranging from 2.5 mm/h to 15 mm/h.

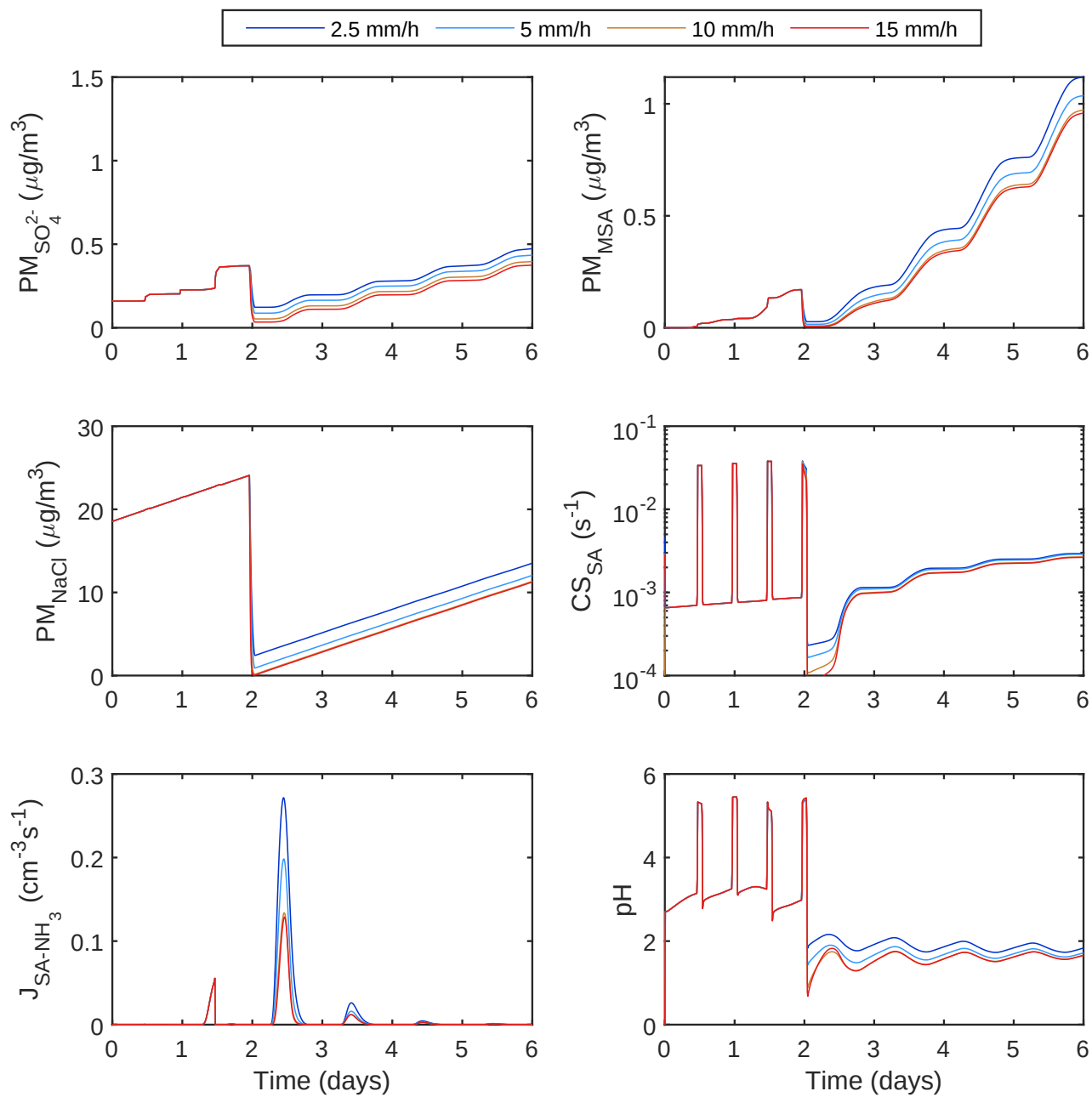


Figure S35. Total SO_4^{2-} , MSA and NaCl PM along with the SA condensation sink, SA-NH₃ driven nucleation rate and bulk pH at varying rates of precipitation ranging from 2.5 mm/h to 15 mm/h.

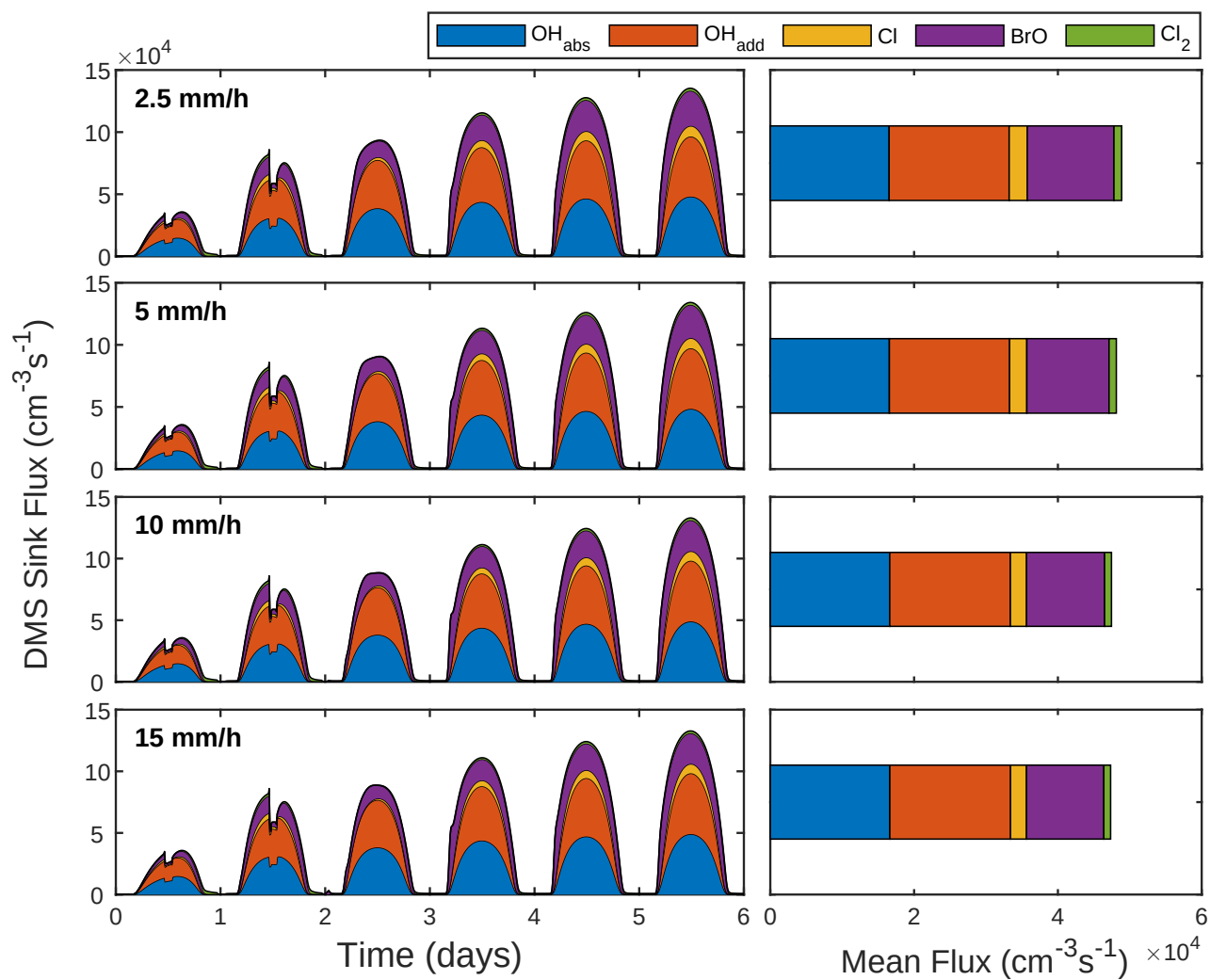


Figure S36. DMS sink flux driven by the reaction with OH (addition), OH (abstraction), Cl, BrO and Cl₂ at varying rates of precipitation ranging from 2.5 mm/h to 15 mm/h. Reactions that contribute < 1% of the total sink flux are not displayed in the figure.

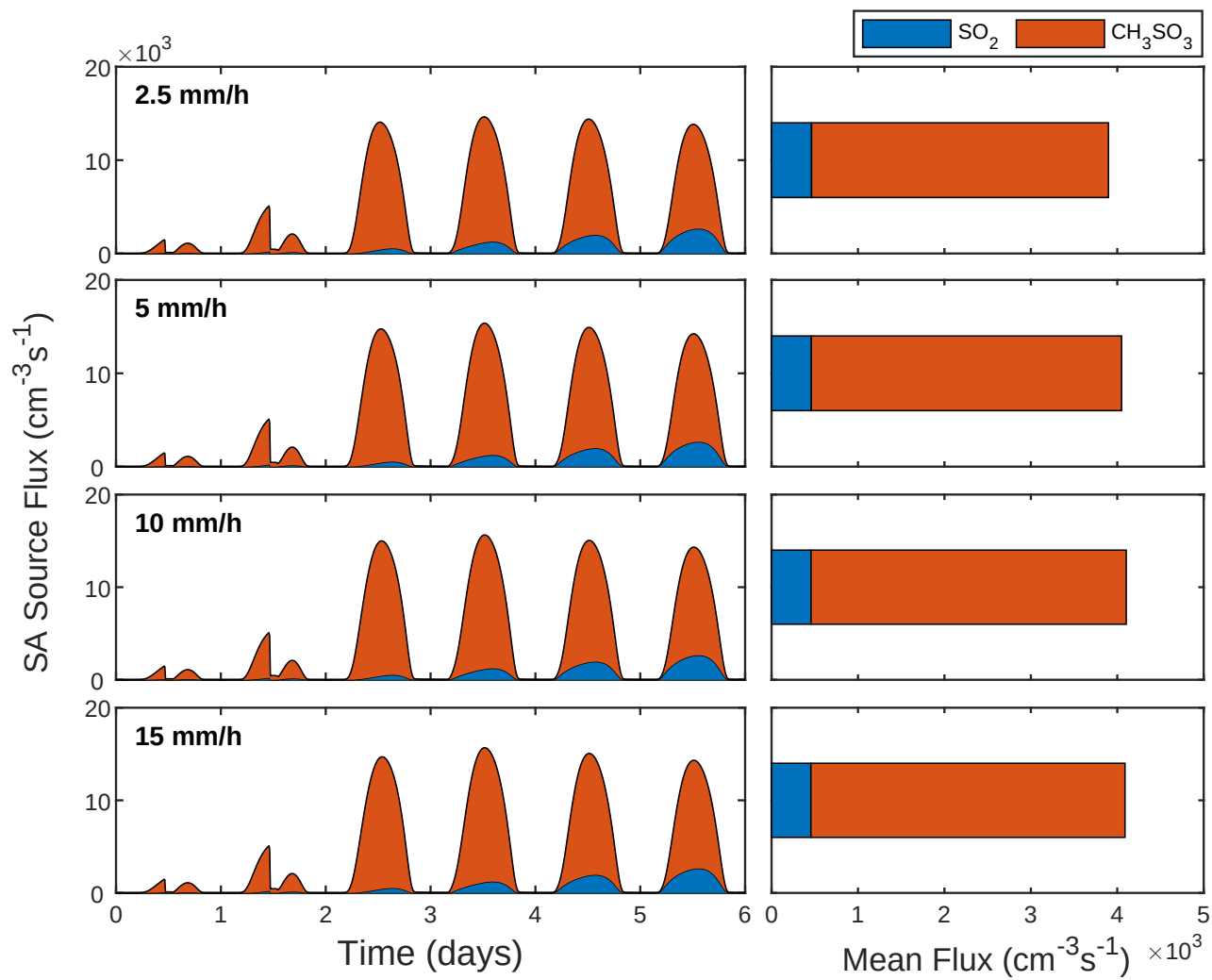


Figure S37. SA source flux from SO_2 and CH_3SO_3 at varying rates of precipitation ranging from 2.5 mm/h to 15 mm/h.

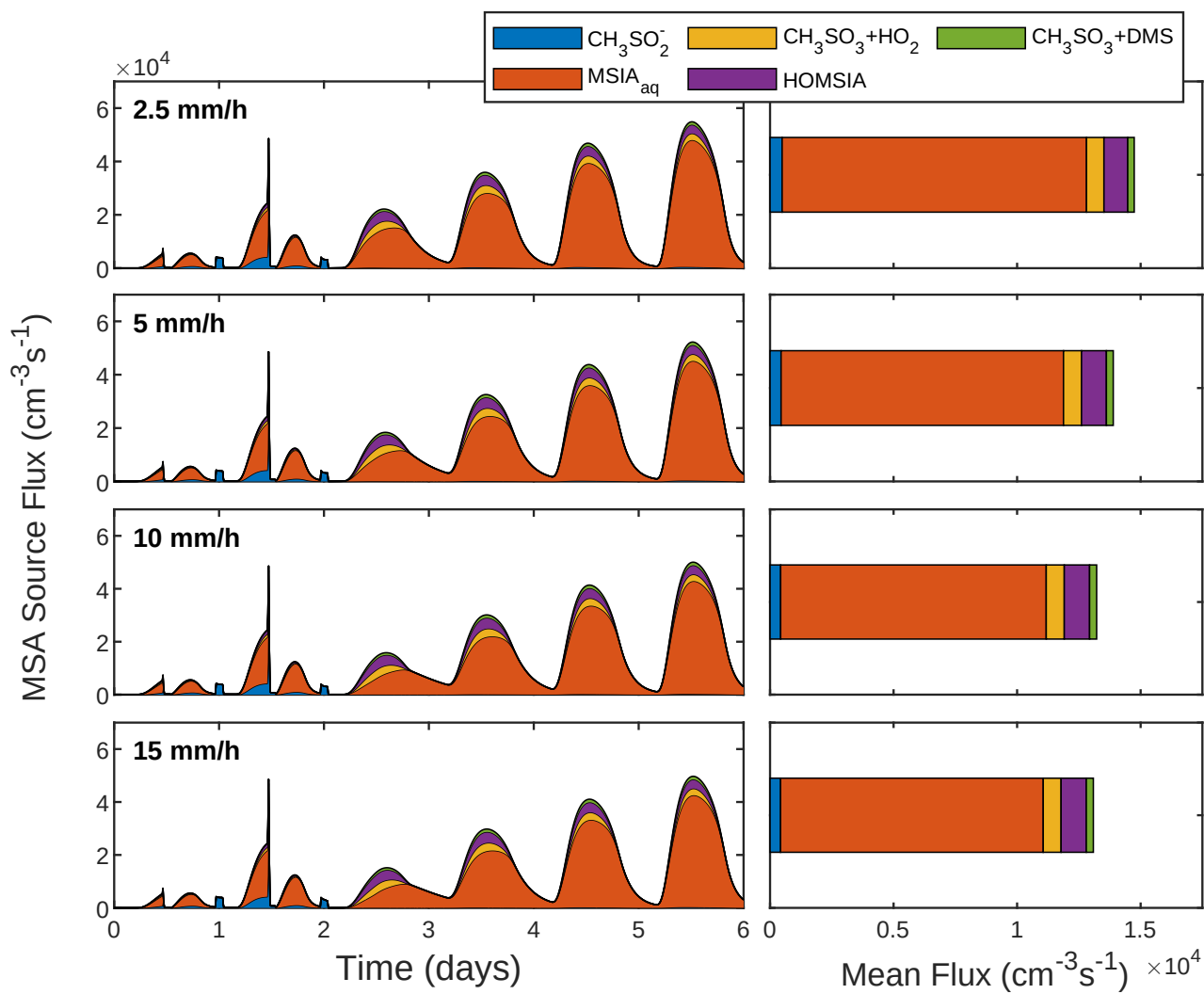


Figure S38. MSA source flux from CH_3SO_2^- and MSIA_{aq} in the aqueous-phase in addition to CH_3SO_3 via HO_2 , CH_3SO_3 via DMS and HOMSA in the gas-phase at varying rates of precipitation ranging from 2.5 mm/h to 15 mm/h.

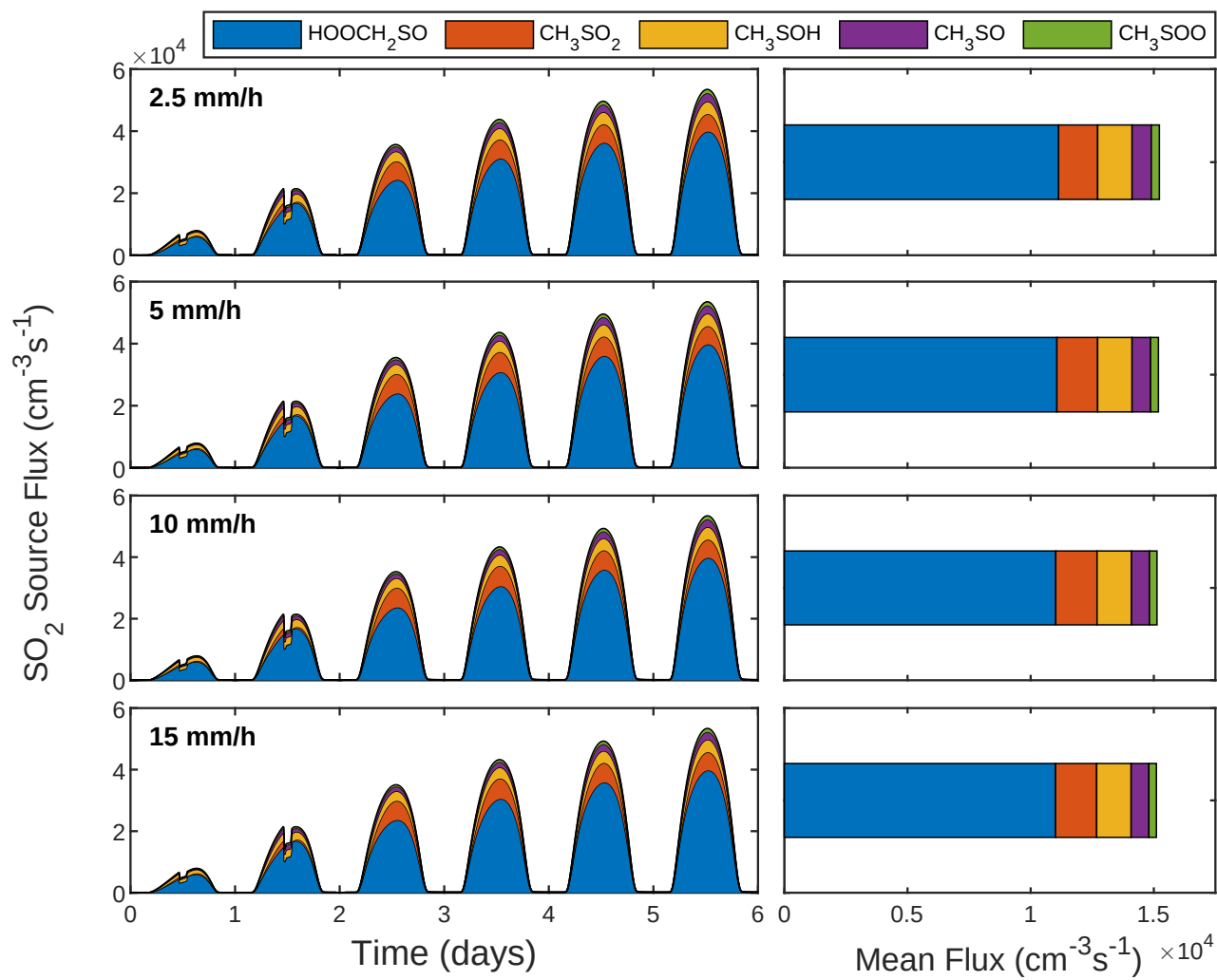


Figure S39. SO₂ source flux from HOOCH₂SO, CH₃SO₂, CH₃SOH, CH₃SO and CH₃SOO at varying rates of precipitation ranging from 2.5 mm/h to 15 mm/h. Reactions that contribute < 1% of the total source flux are not displayed in the figure.

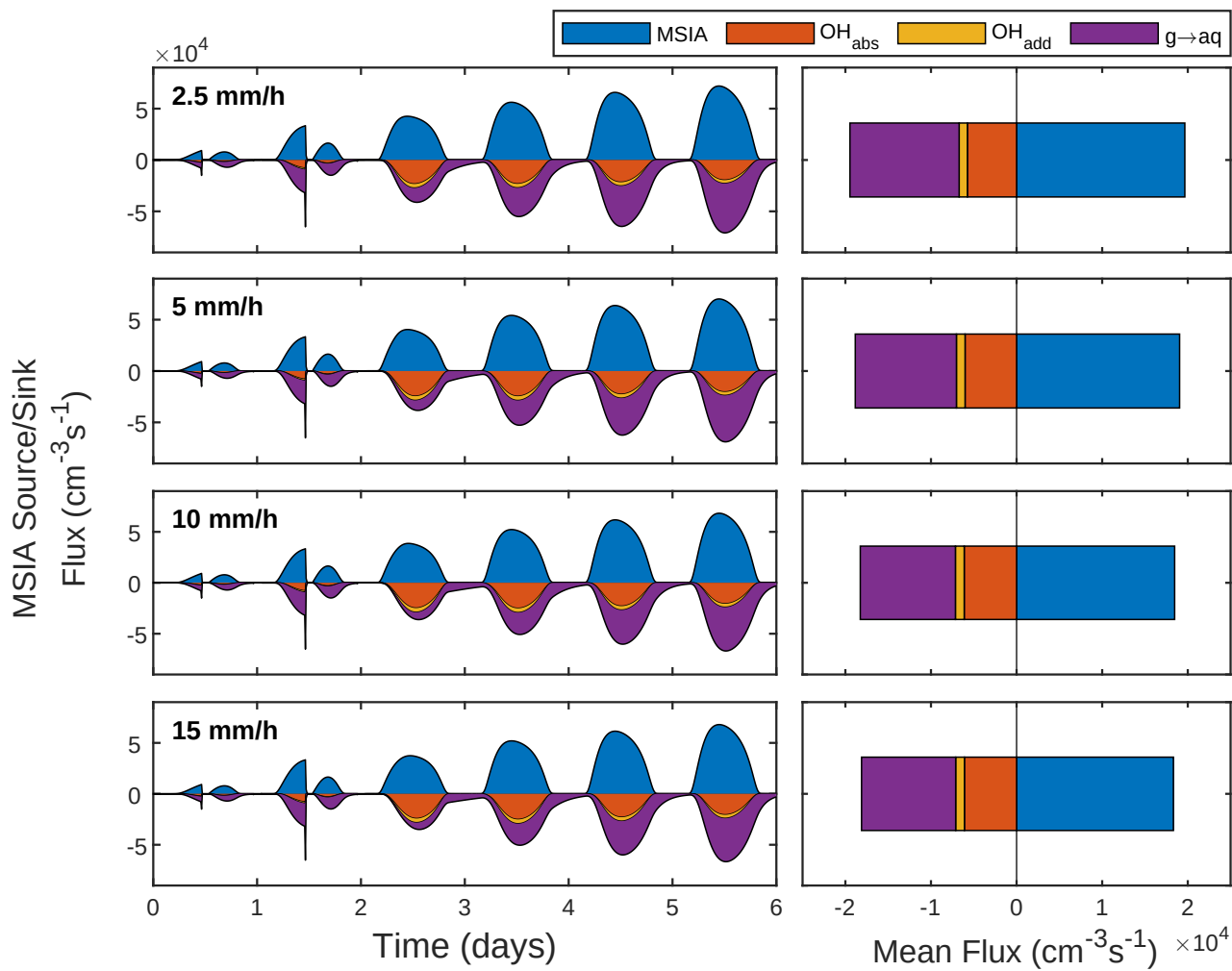


Figure S40. MSIA source/sink flux from DMSO and via reaction with OH (abstraction), OH (addition) and gas-aqueous phase uptake at varying rates of precipitation ranging from 2.5 mm/h to 15 mm/h. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

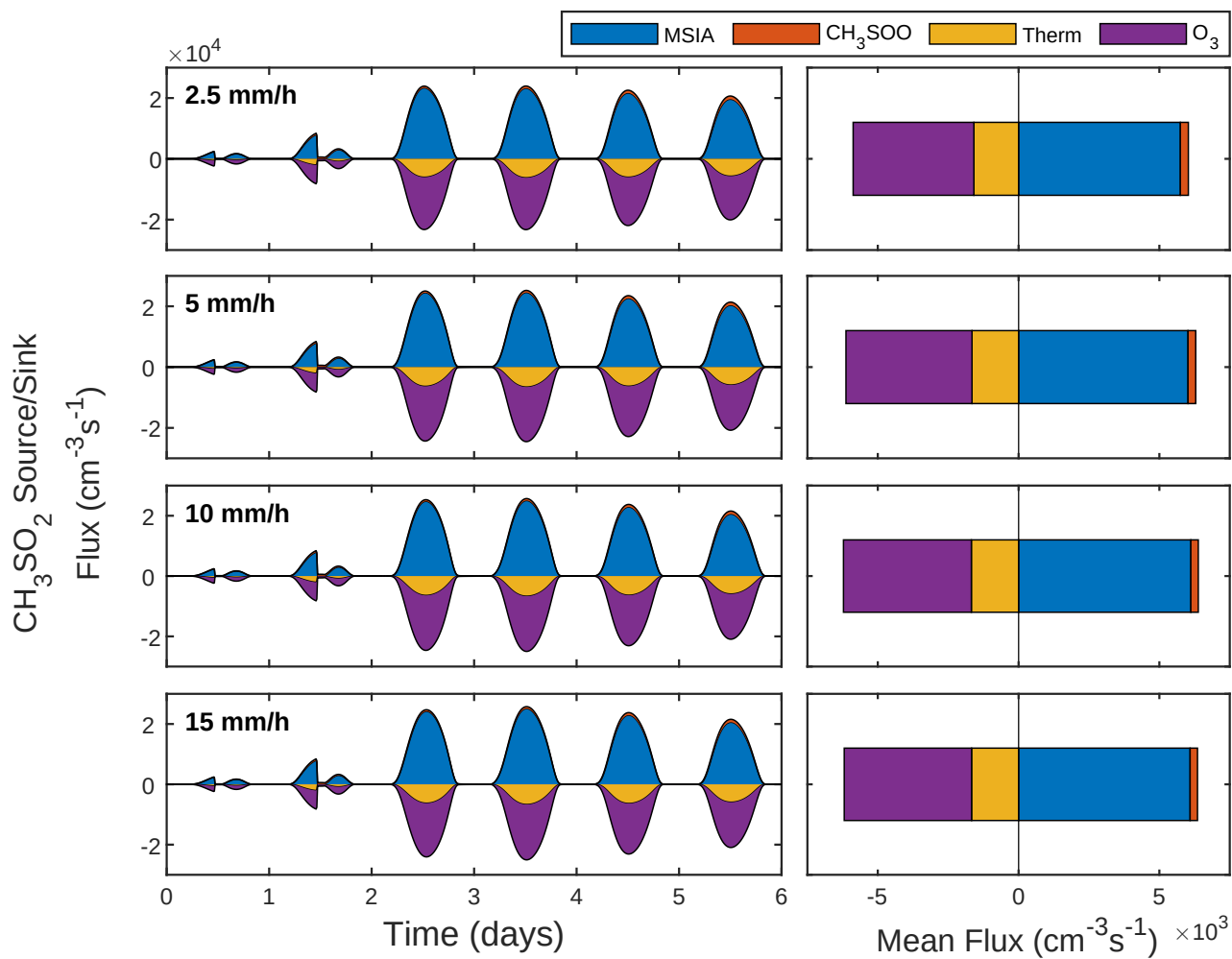


Figure S41. CH_3SO_2 source/sink flux from MSIA, CH_3SOO and via thermal decomposition and reaction with O_3 at varying rates of precipitation ranging from 2.5 mm/h to 15 mm/h. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

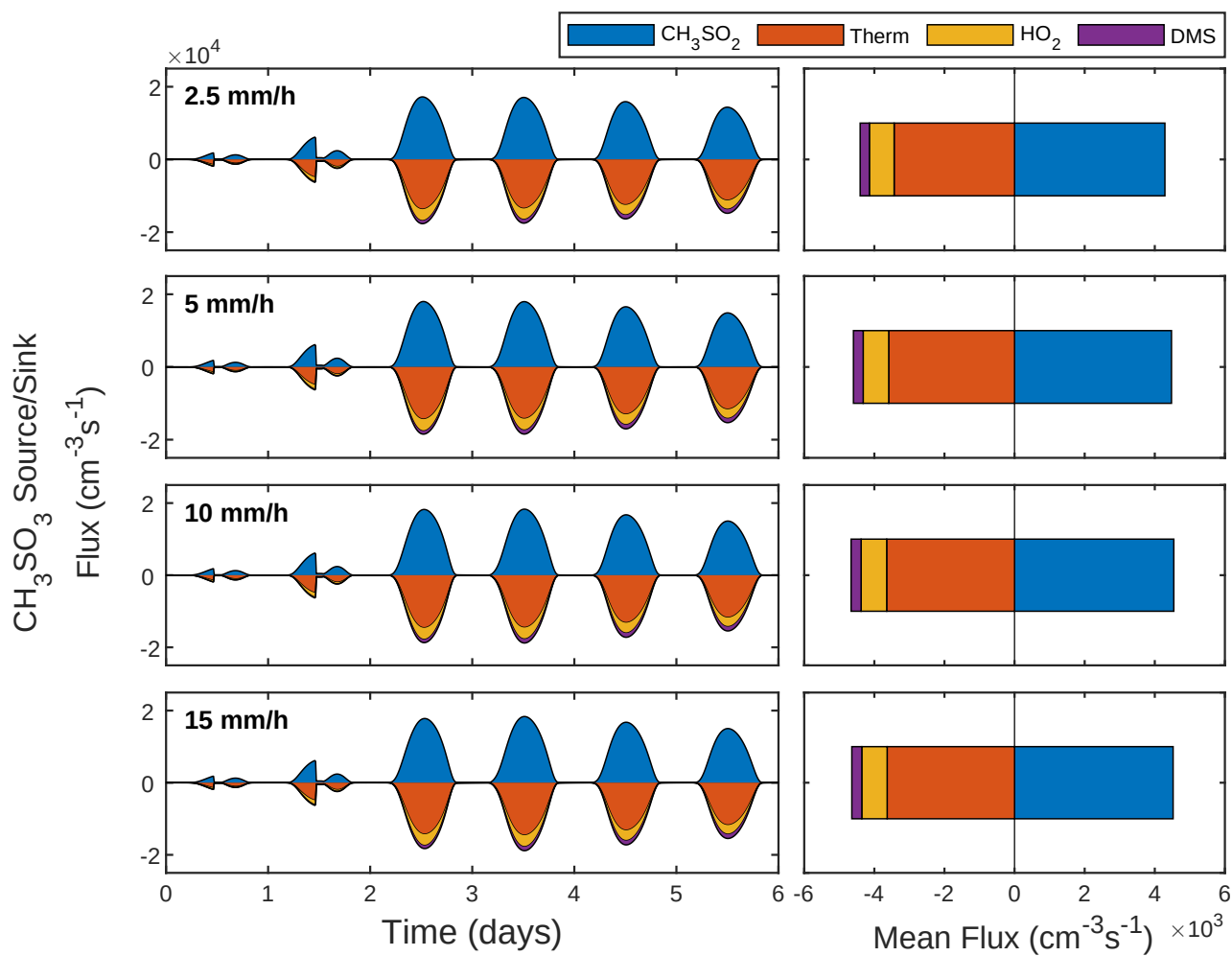


Figure S42. CH_3SO_3 source/sink flux from CH_3SO_2 , via thermal decomposition and reaction with HO_2 and DMS at varying rates of precipitation ranging from 2.5 mm/h to 15 mm/h. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

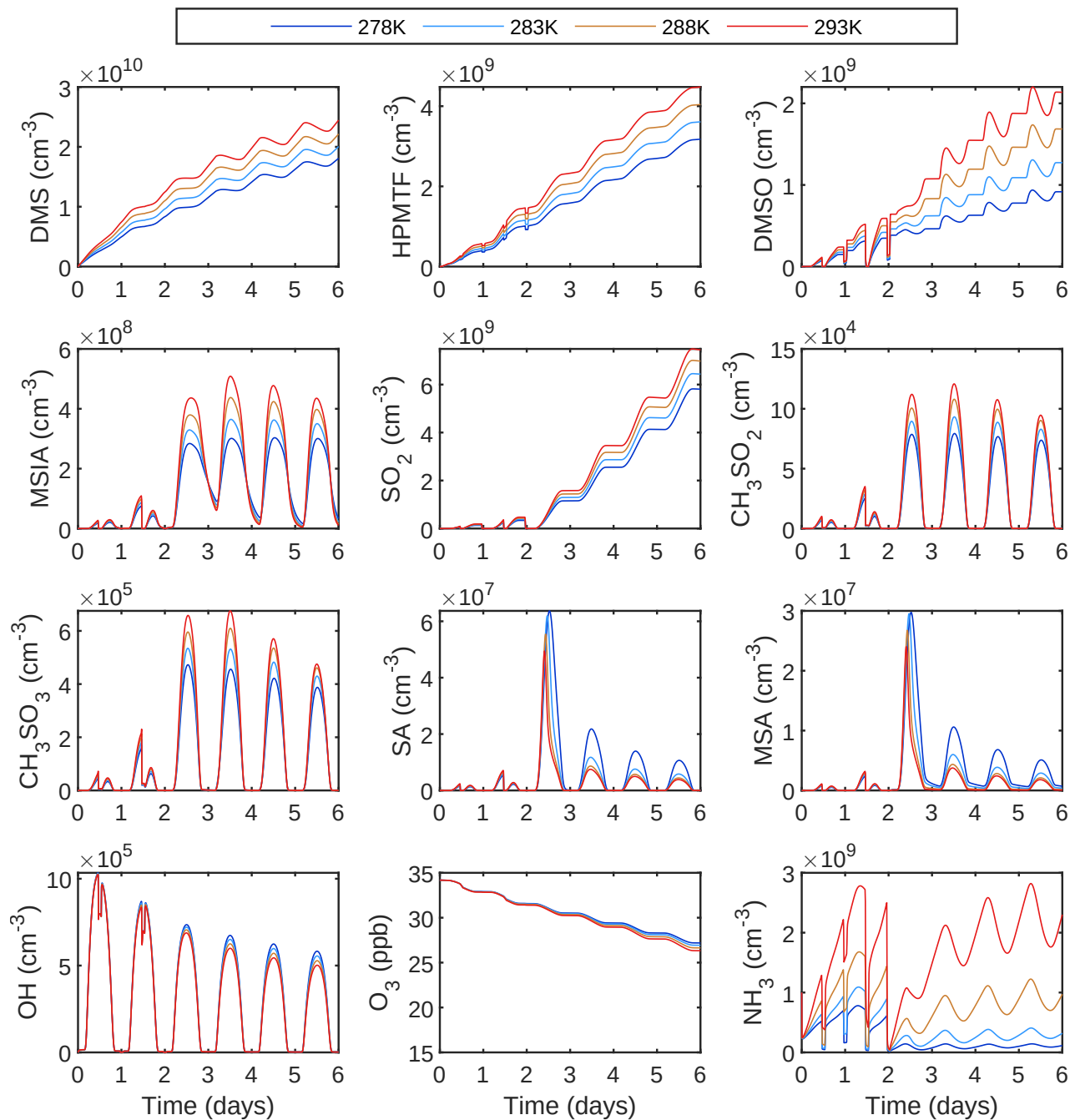


Figure S43. Concentrations of key gas-phase species at varying sea surface temperatures ranging from 278 K to 293 K.

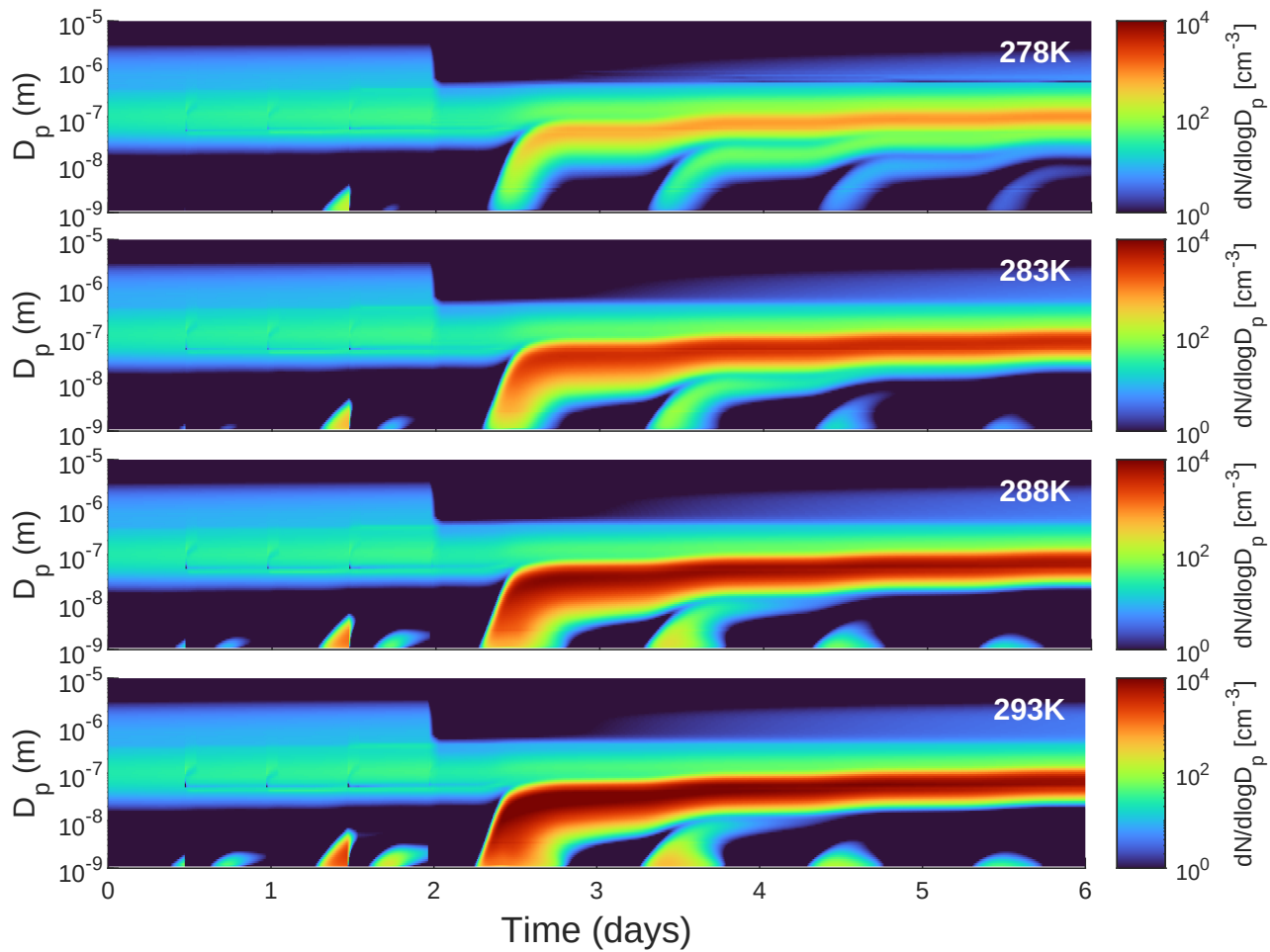


Figure S44. Aerosol particle number size distributions throughout the full simulation period at varying sea surface temperatures ranging from 278 K to 293 K.

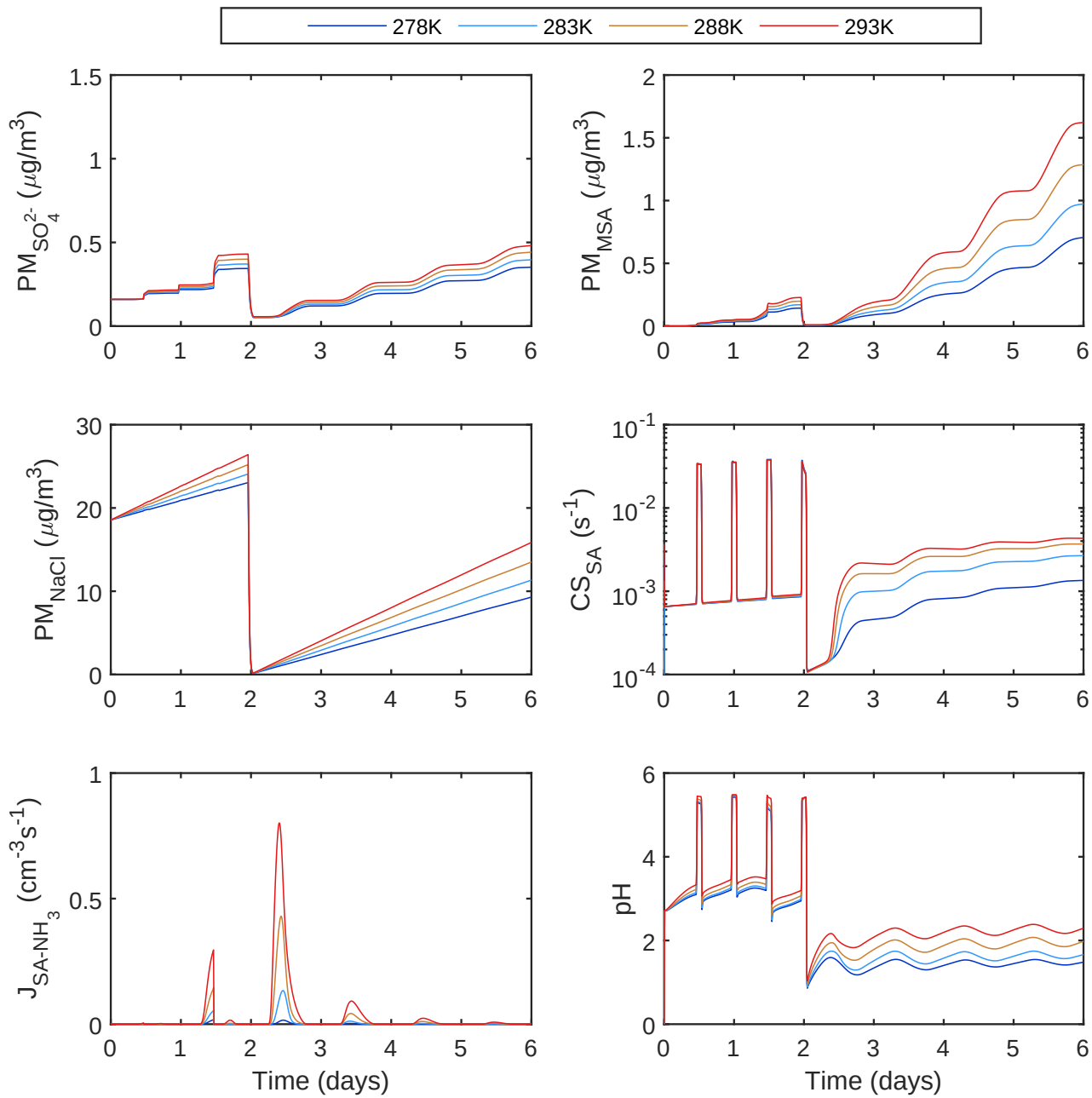


Figure S45. Total SO_4^{2-} , MSA and NaCl PM along with the SA condensation sink, SA-NH₃ driven nucleation rate and bulk pH at varying sea surface temperatures ranging from 278 K to 293 K.

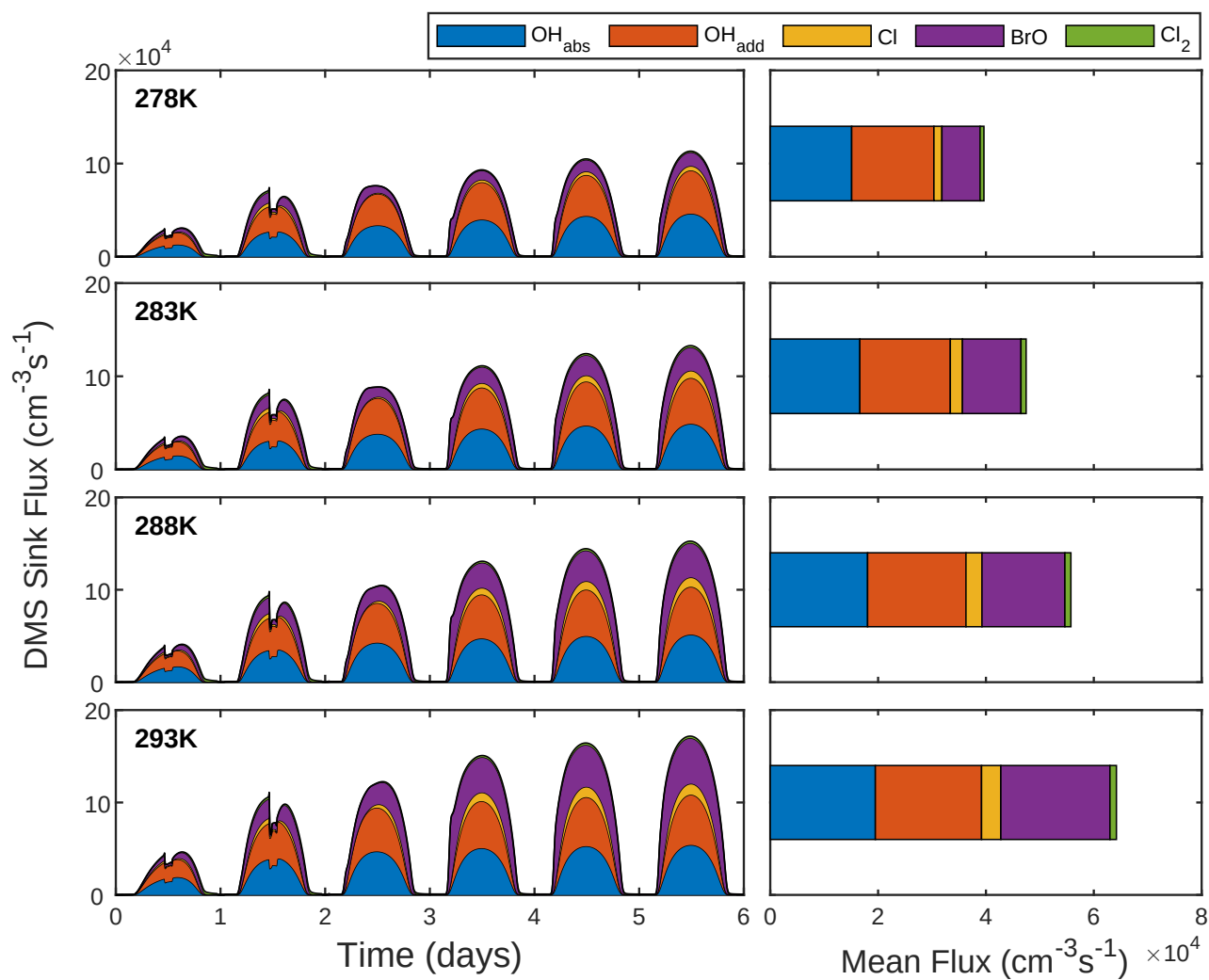


Figure S46. DMS sink flux driven by the reaction with OH (addition), OH (abstraction), Cl, BrO and Cl₂ at varying sea surface temperatures ranging from 278 K to 293 K. Reactions that contribute < 1% of the total sink flux are not displayed in the figure.

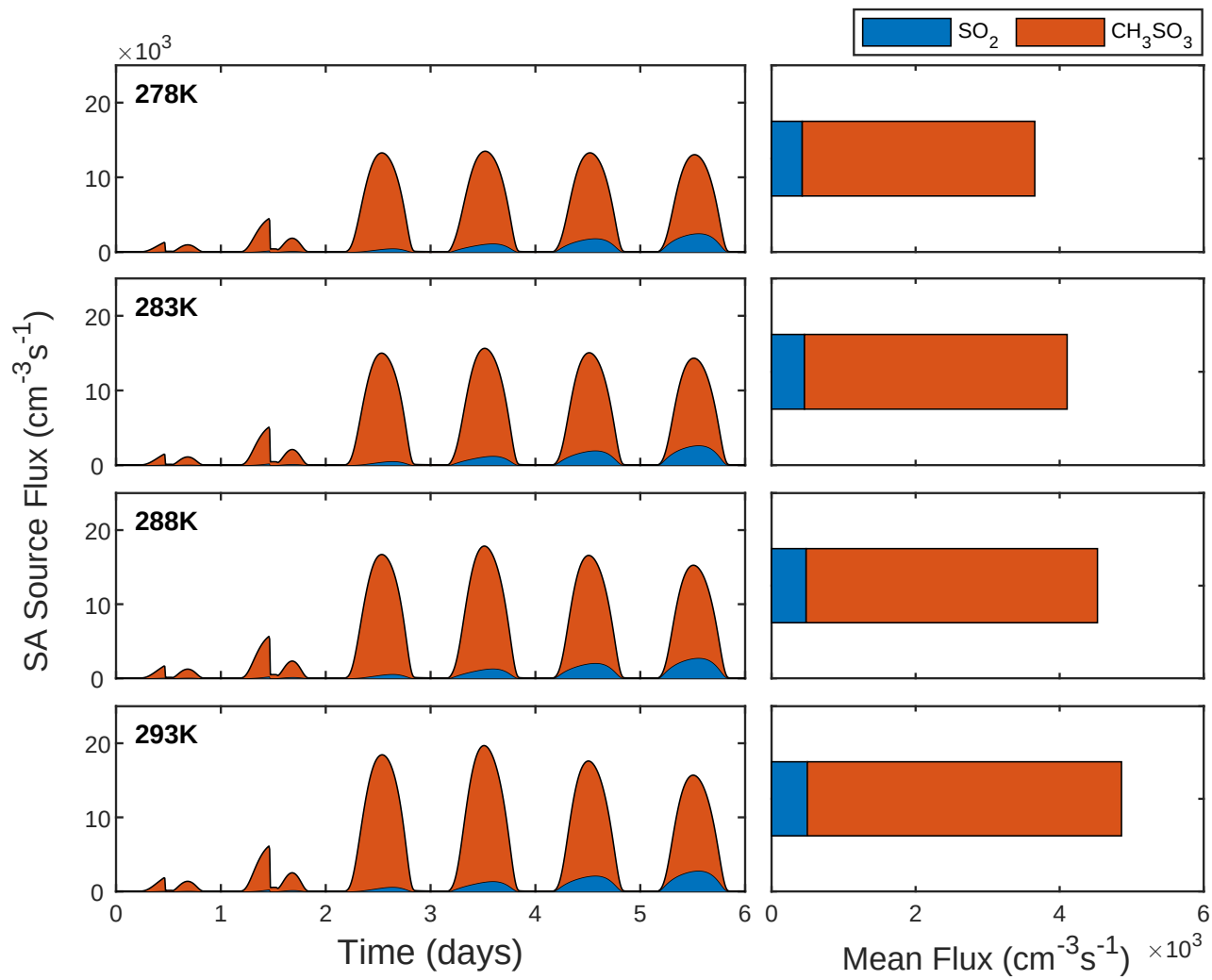


Figure S47. SA source flux from SO_2 and CH_3SO_3 at varying sea surface temperatures ranging from 278 K to 293 K

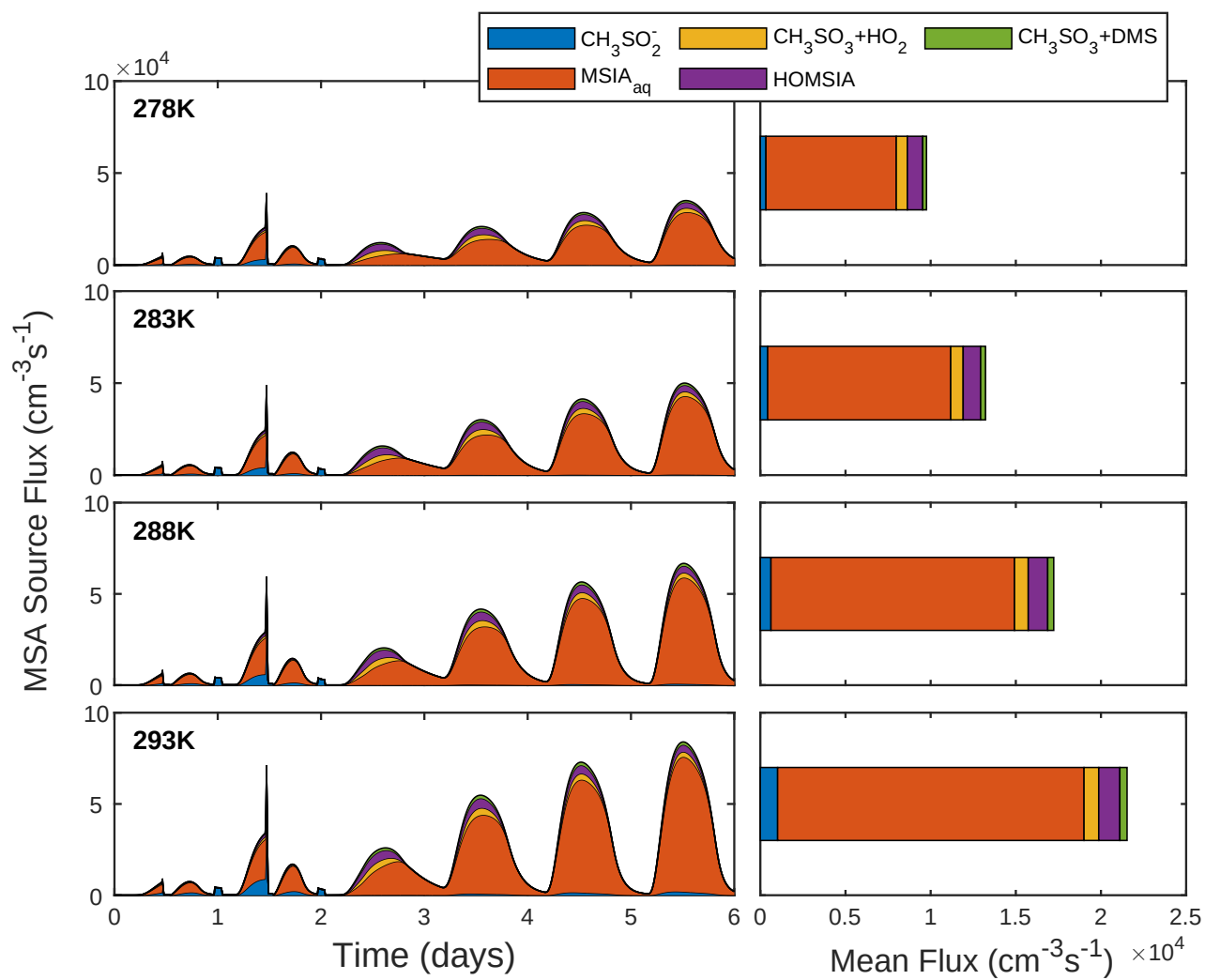


Figure S48. MSA source flux from CH_3SO_2^- and MSIA_{aq} in the aqueous-phase in addition to CH_3SO_3 via HO_2 , CH_3SO_3 via DMS and HOMSA in the gas-phase at varying sea surface temperatures ranging from 278 K to 293 K.

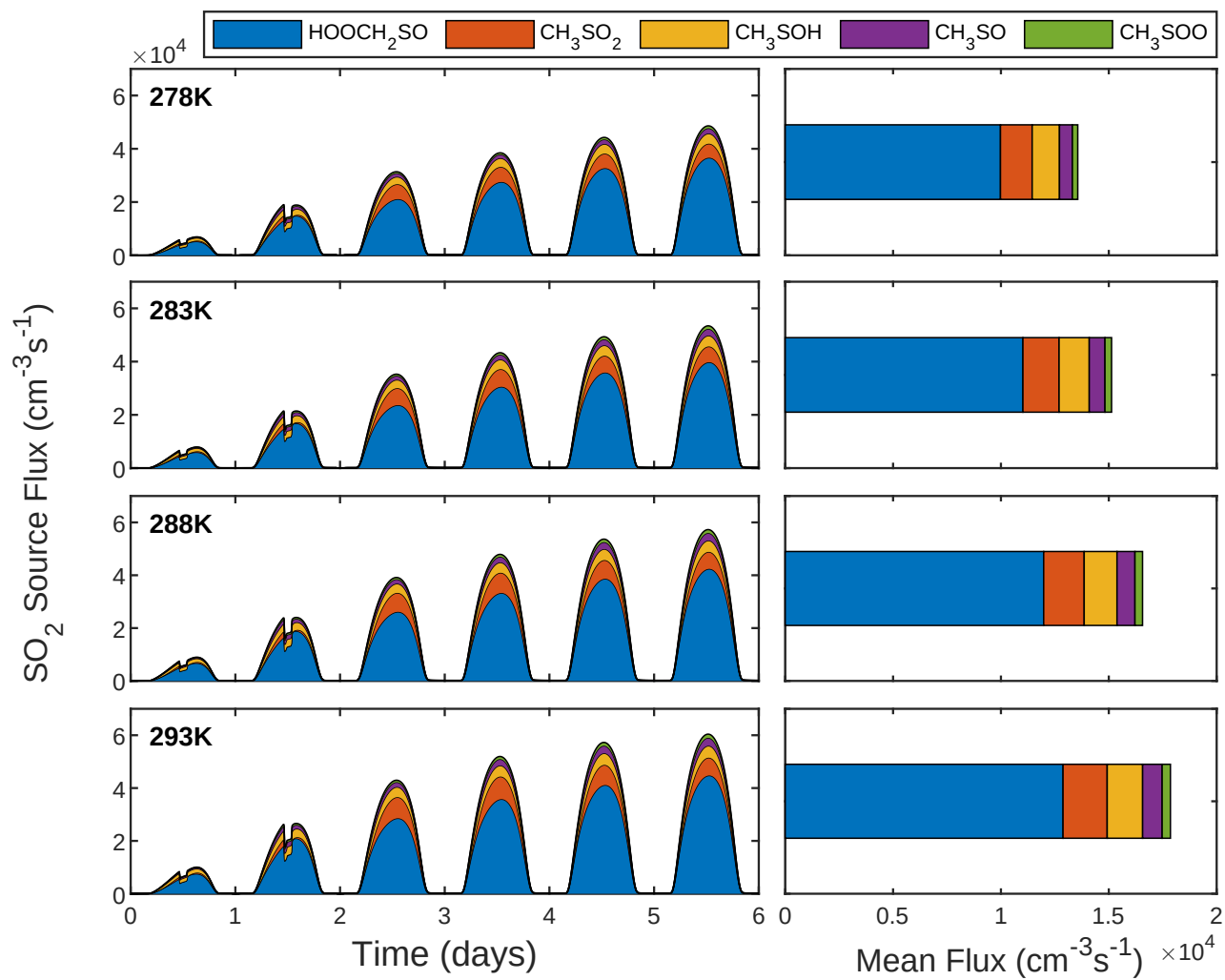


Figure S49. SO₂ source flux from HOOCH₂SO, CH₃SO₂, CH₃SOH, CH₃SO and CH₃SOO at varying sea surface temperatures ranging from 278 K to 293 K. Reactions that contribute < 1% of the total source flux are not displayed in the figure.

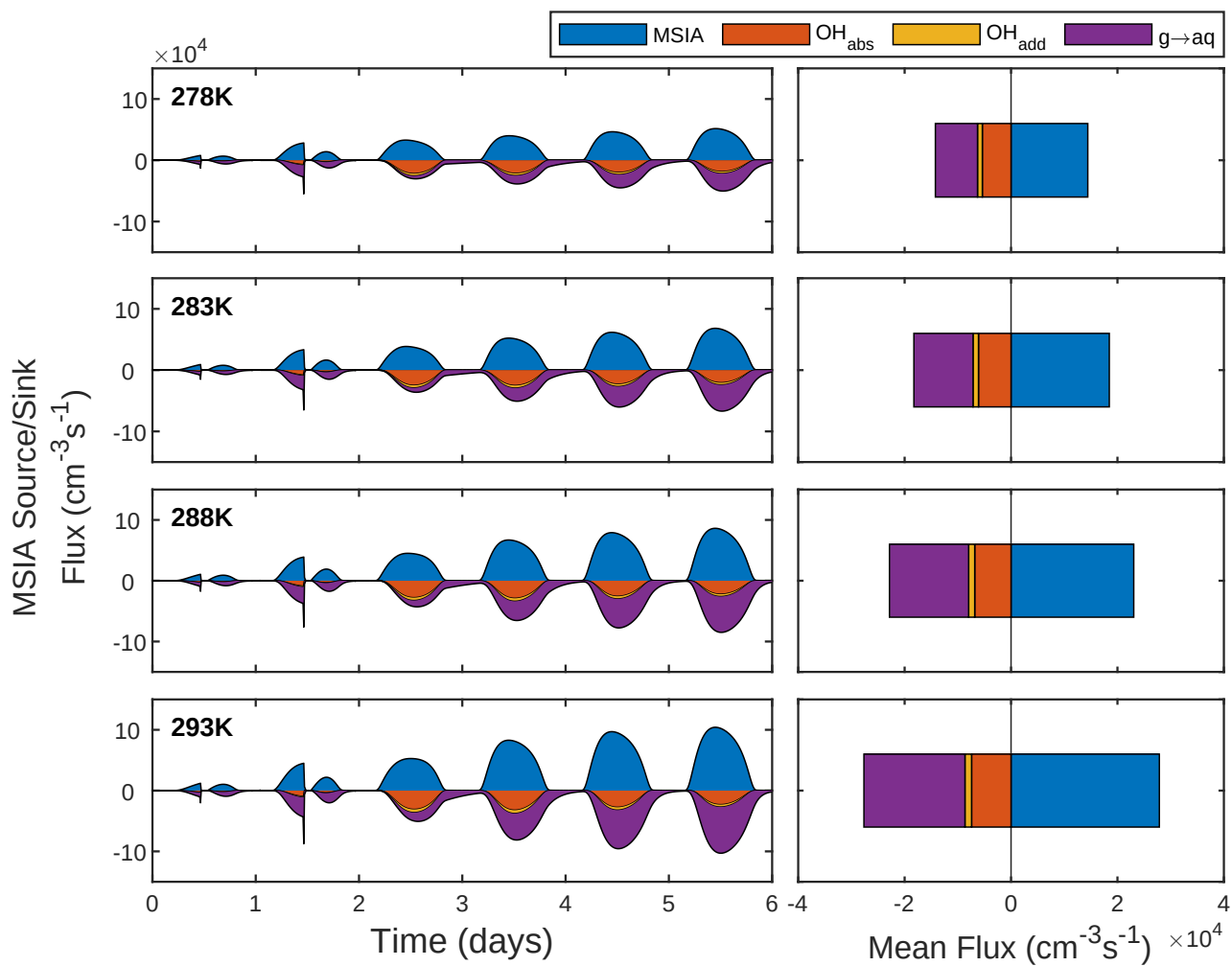


Figure S50. MSIA source/sink flux from DMSO and via reaction with OH (abstraction), OH (addition) and gas-aqueous phase uptake at varying sea surface temperatures ranging from 278 K to 293 K. Reactions that contribute $< 1\%$ of the total source/sink flux are not displayed in the figure.

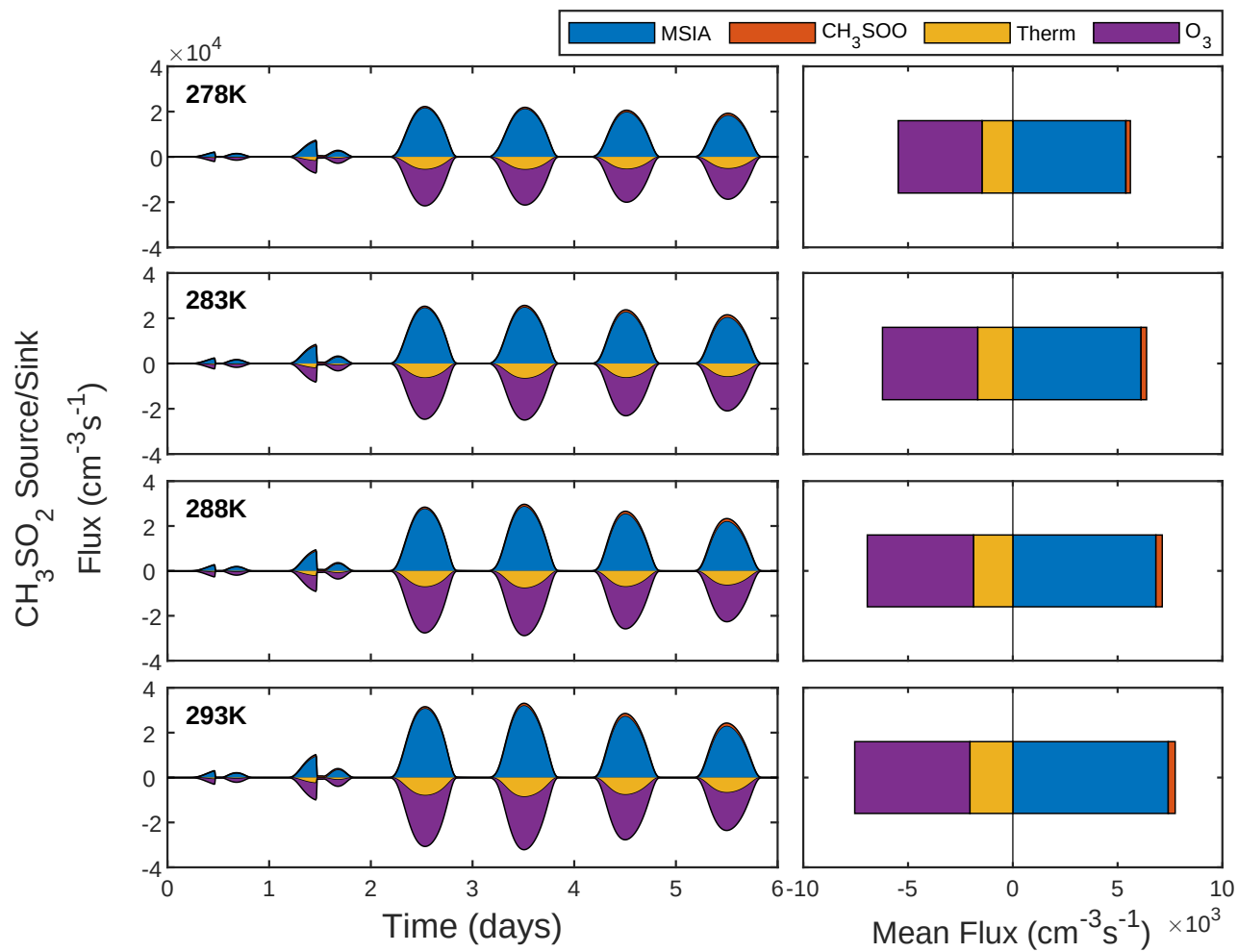


Figure S51. CH_3SO_2 source/sink flux from MSIA, CH_3SOO and via thermal decomposition and reaction with O_3 at varying sea surface temperatures ranging from 278 K to 293 K. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

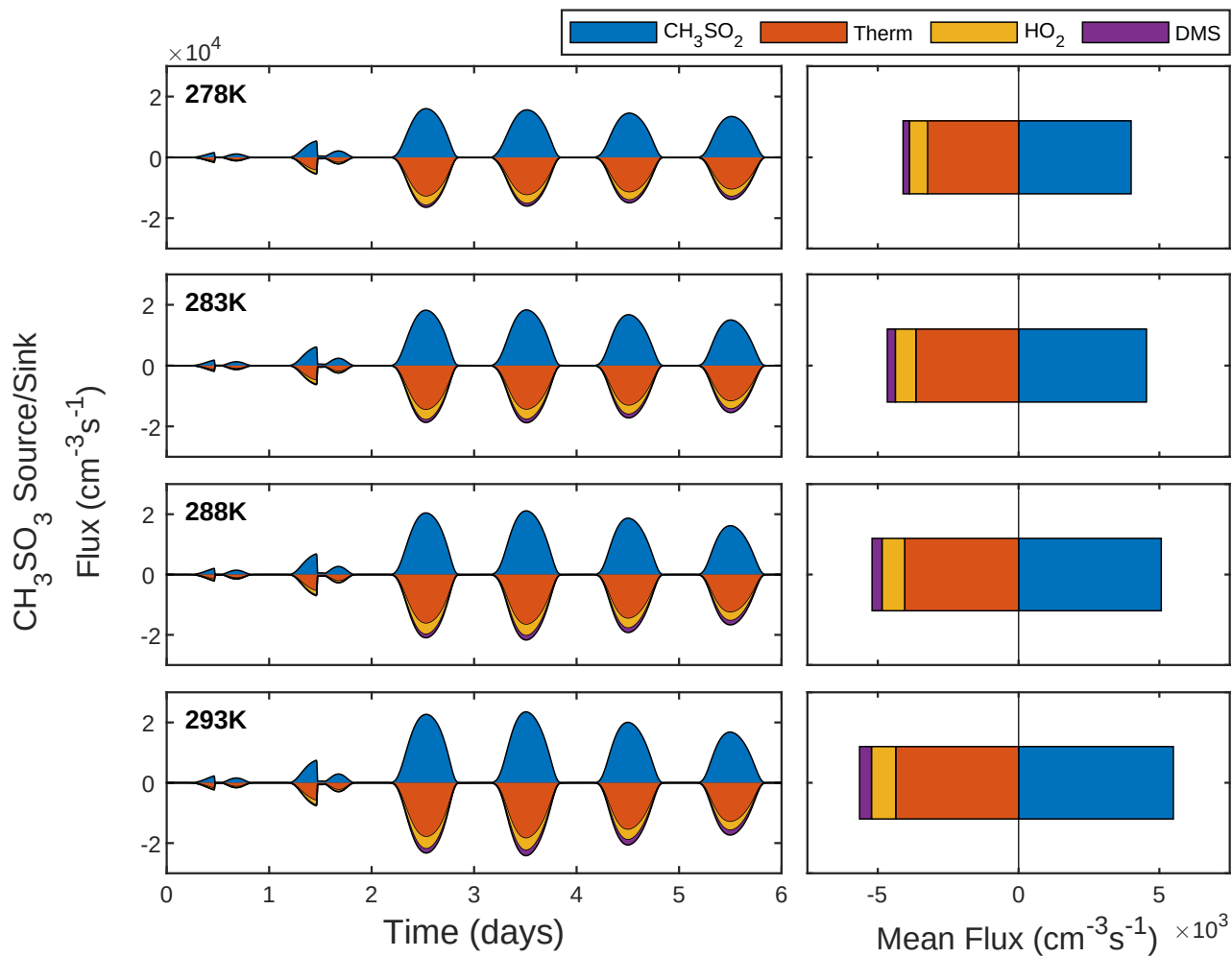


Figure S52. CH_3SO_3 source/sink flux from CH_3SO_2 , via thermal decomposition and reaction with HO_2 and DMS at varying sea surface temperatures ranging from 278 K to 293 K. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

S10 DMS sea surface concentration sensitivity runs

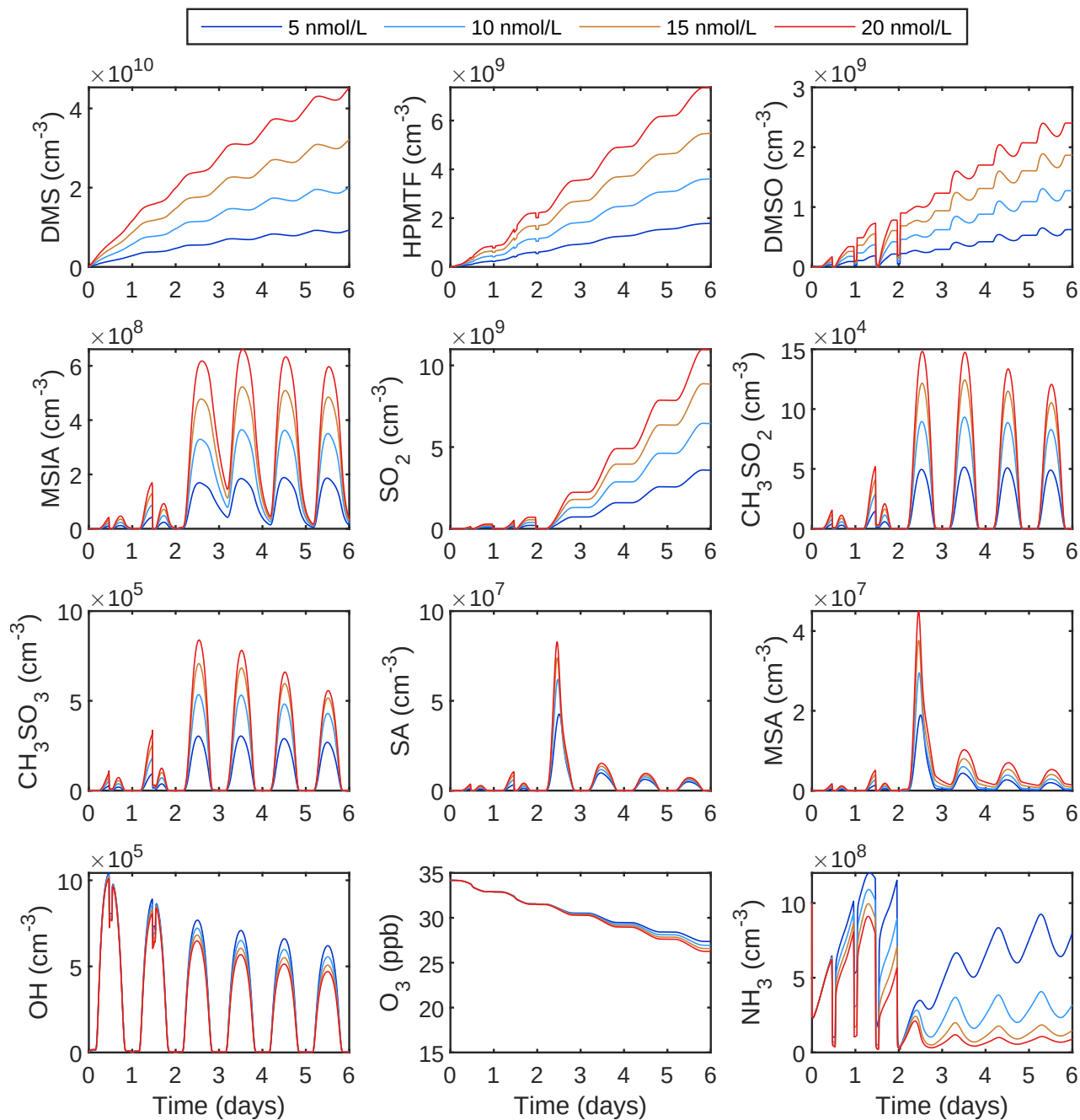


Figure S53. Concentrations of key gas-phase species at varying DMS sea surface concentrations ranging from 5 nM to 20 nM.

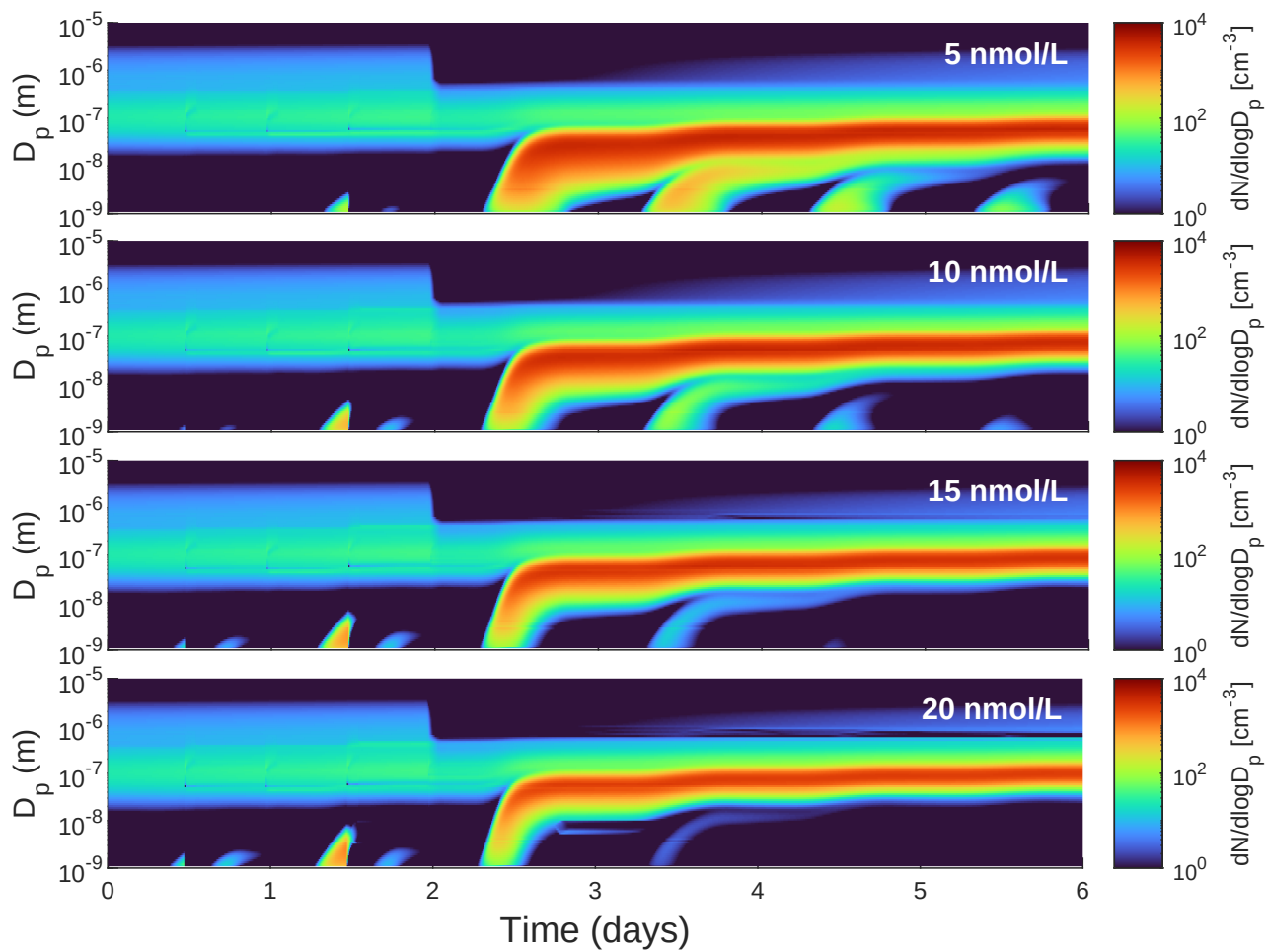


Figure S54. Aerosol particle number size distributions throughout the full simulation period at varying DMS sea surface concentrations ranging from 5 nM to 20 nM.

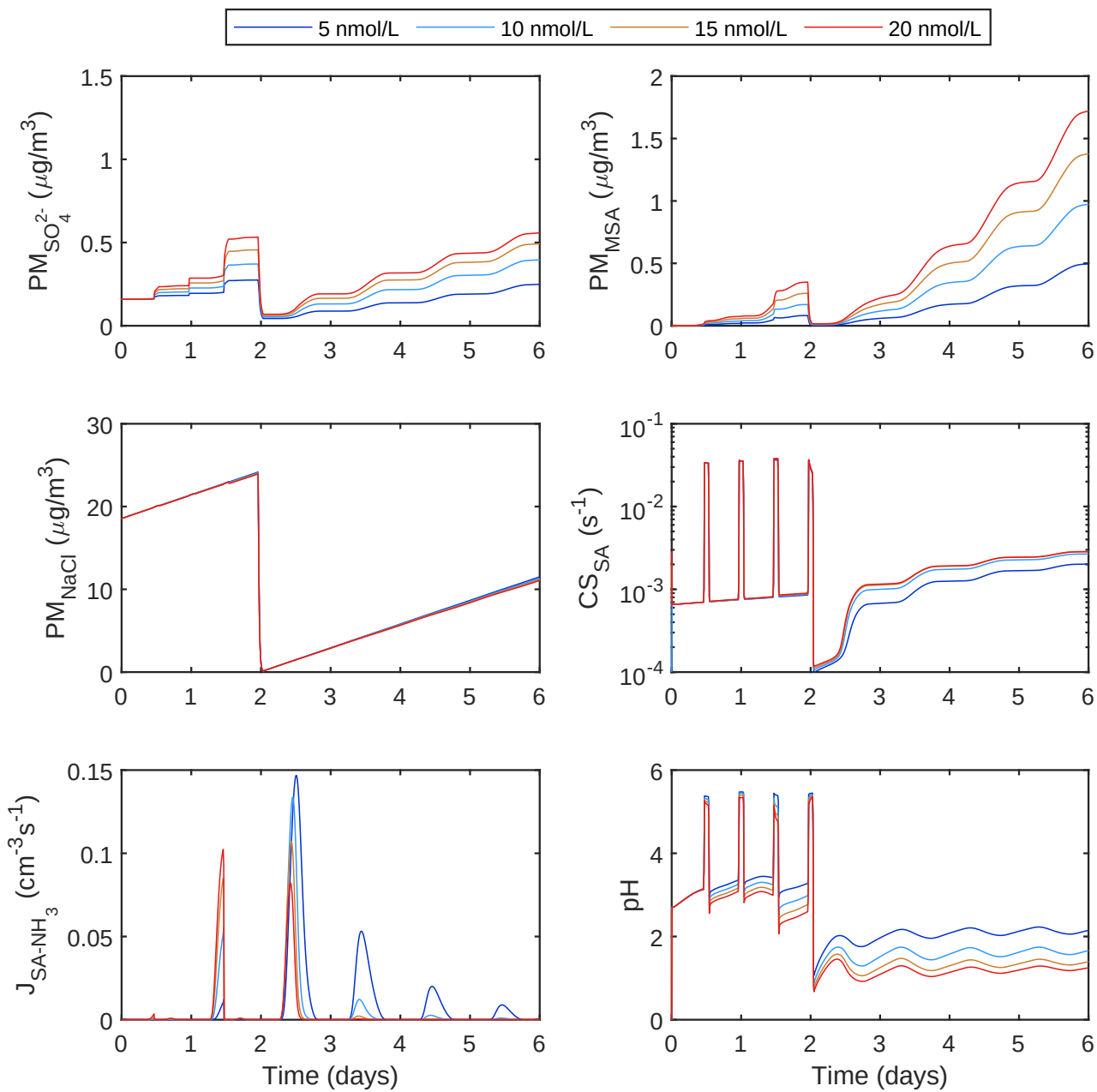


Figure S55. Total SO_4^{2-} , MSA and NaCl PM along with the SA condensation sink, SA- NH_3 driven nucleation rate and bulk pH at varying DMS sea surface concentrations ranging from 5 nM to 20 nM.

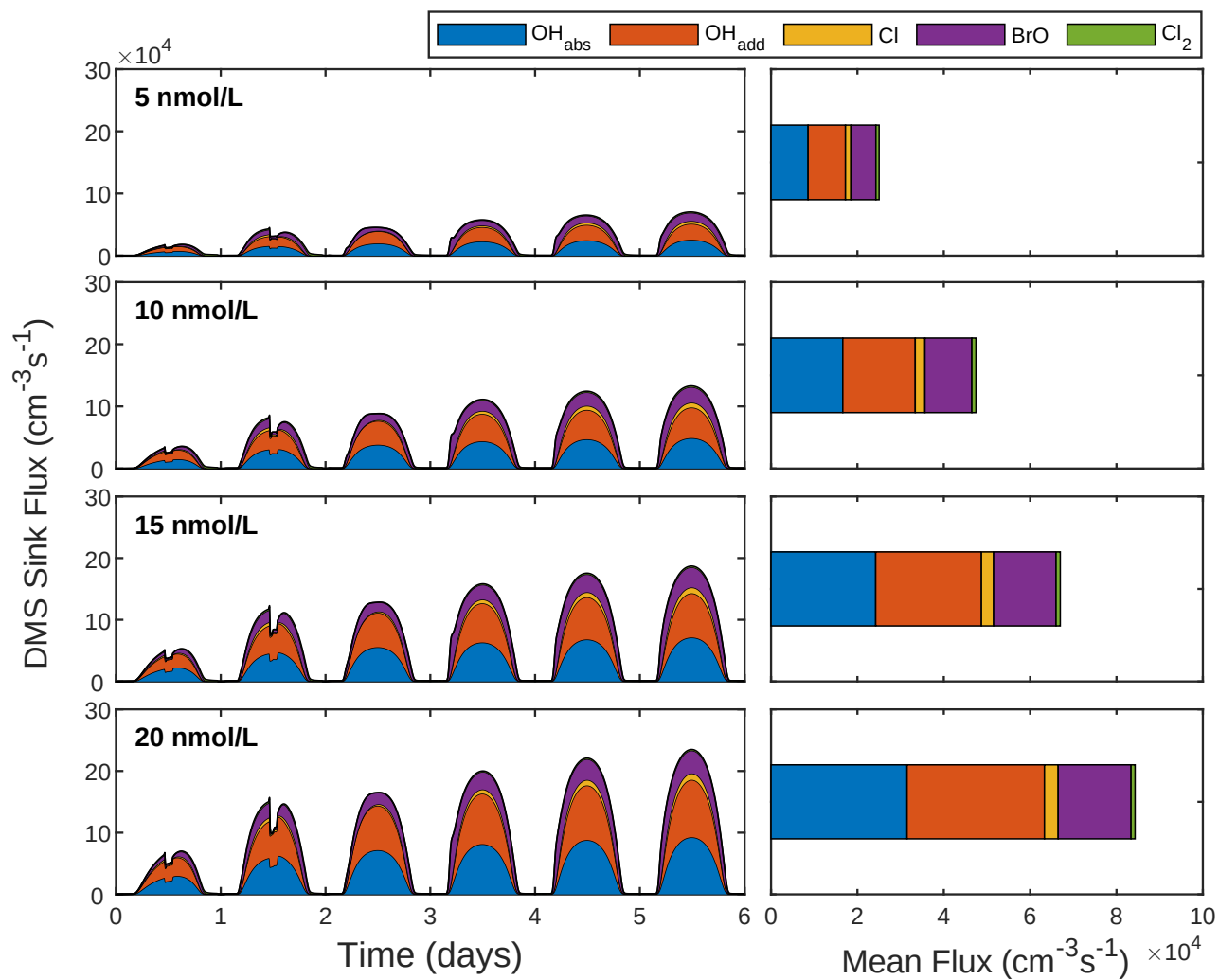


Figure S56. DMS sink flux driven by the reaction with OH (addition), OH (abstraction), Cl, BrO and Cl₂ at varying DMS sea surface concentrations ranging from 5 nM to 20 nM. Reactions that contribute < 1% of the total sink flux are not displayed in the figure.

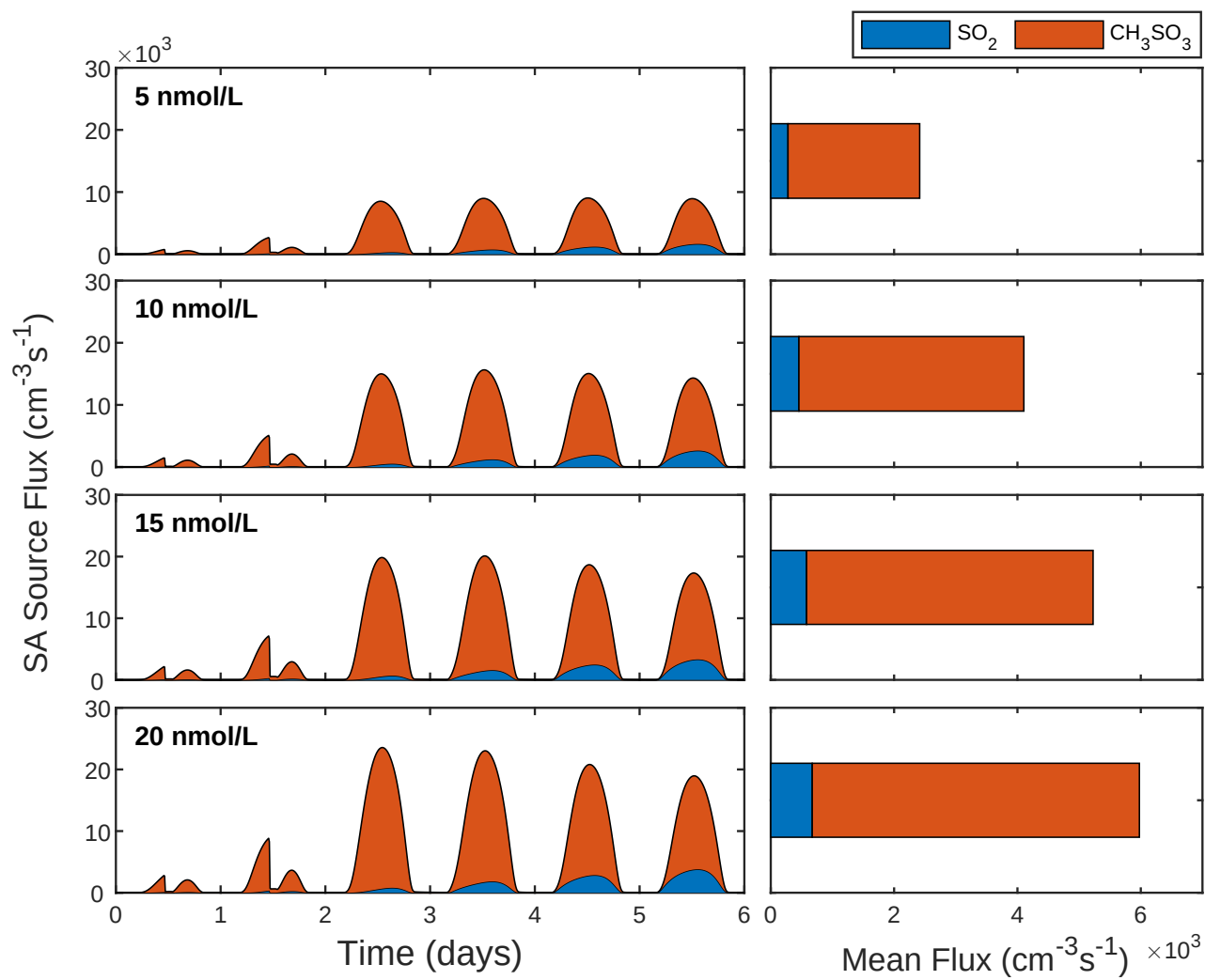


Figure S57. SA source flux from SO_2 and CH_3SO_3 at varying DMS sea surface concentrations ranging from 5 nM to 20 nM.

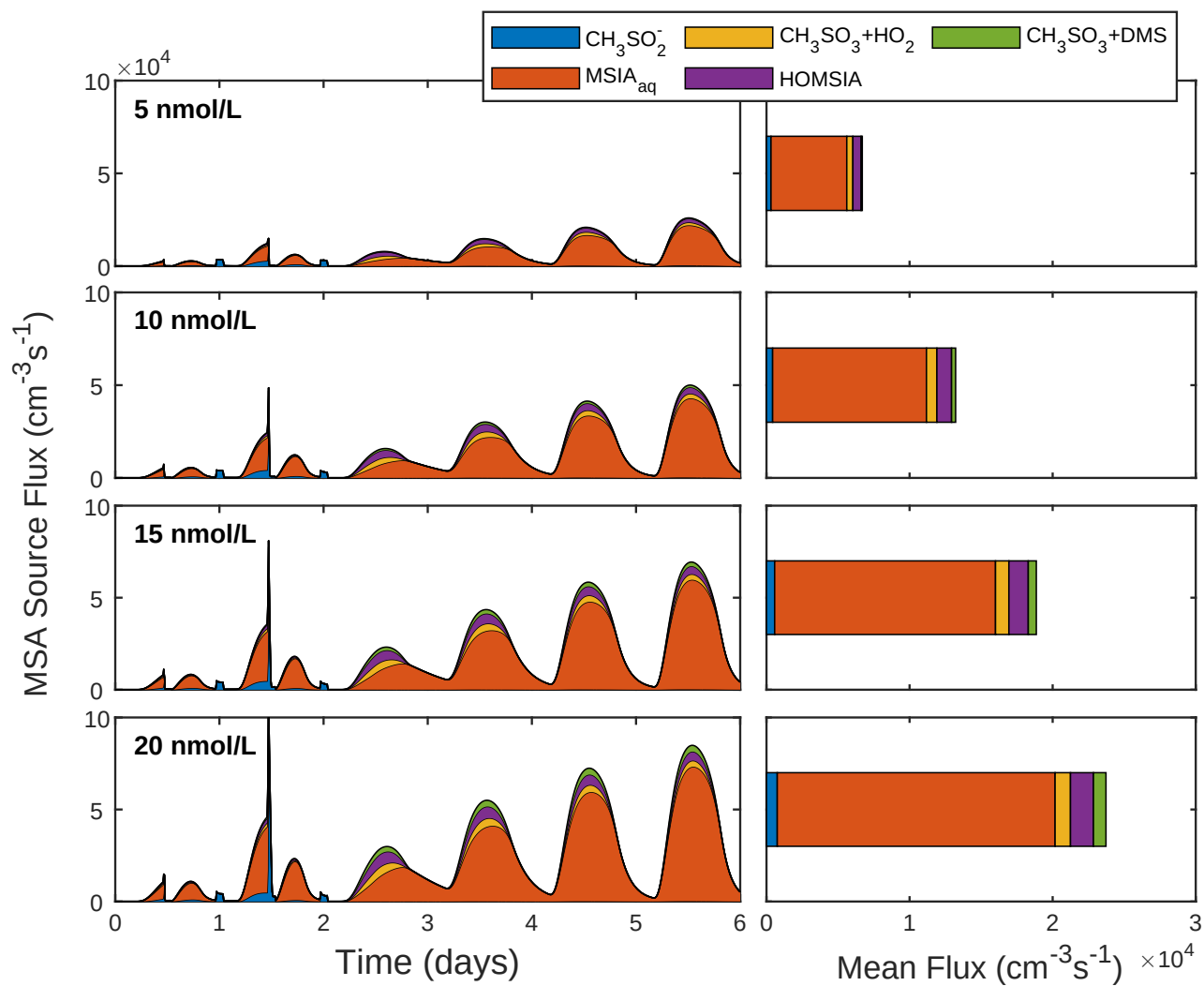


Figure S58. MSA source flux from CH_3SO_2^- and MSIA_{aq} in the aqueous-phase in addition to CH_3SO_3 via HO_2 , CH_3SO_3 via DMS and HOMSIA in the gas-phase at varying DMS sea surface concentrations ranging from 5 nM to 20 nM.

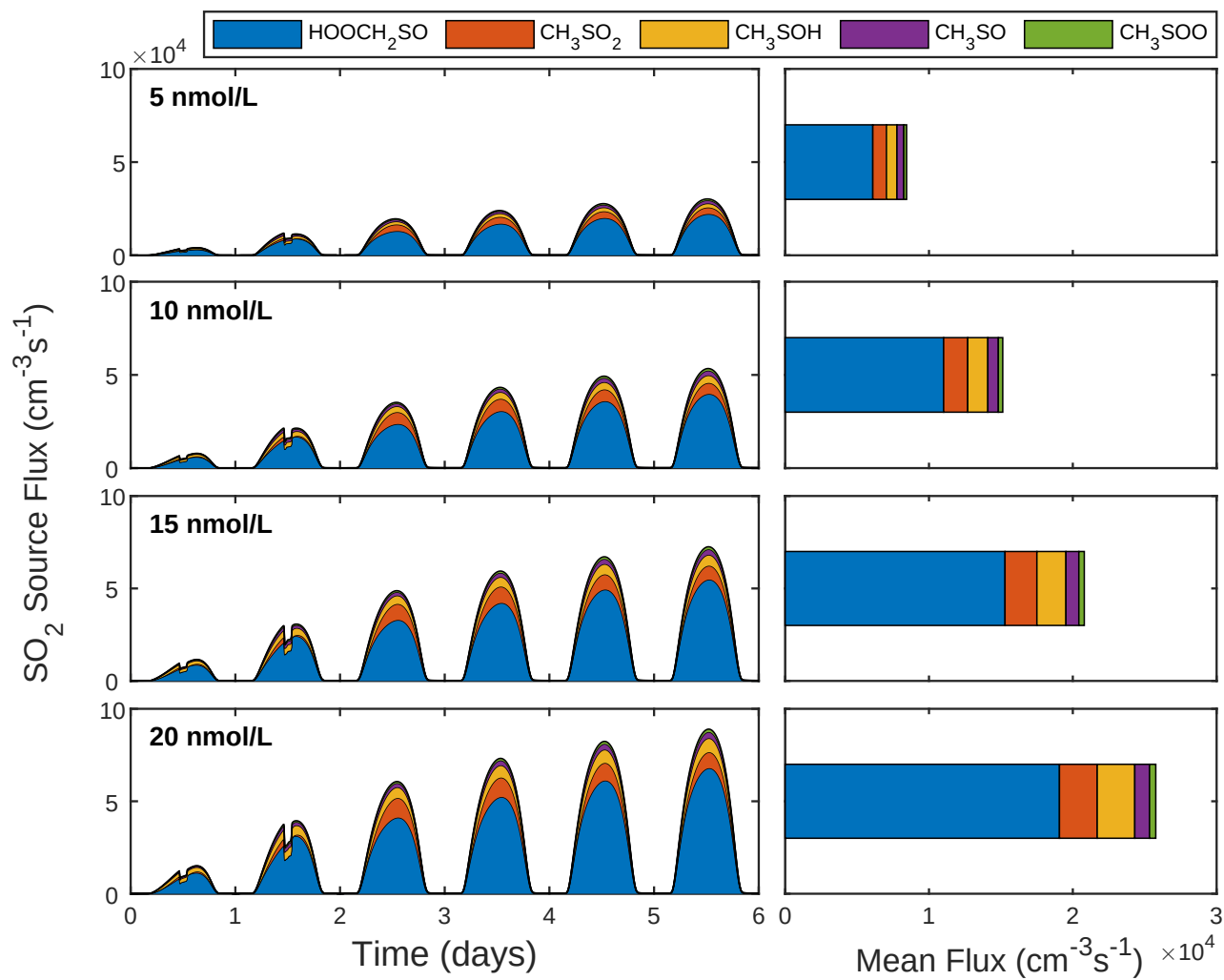


Figure S59. SO_2 source flux from HOOCH_2SO , CH_3SO_2 , CH_3SOH , CH_3SO and CH_3SOO at varying DMS sea surface concentrations ranging from 5 nM to 20 nM. Reactions that contribute < 1% of the total source flux are not displayed in the figure.

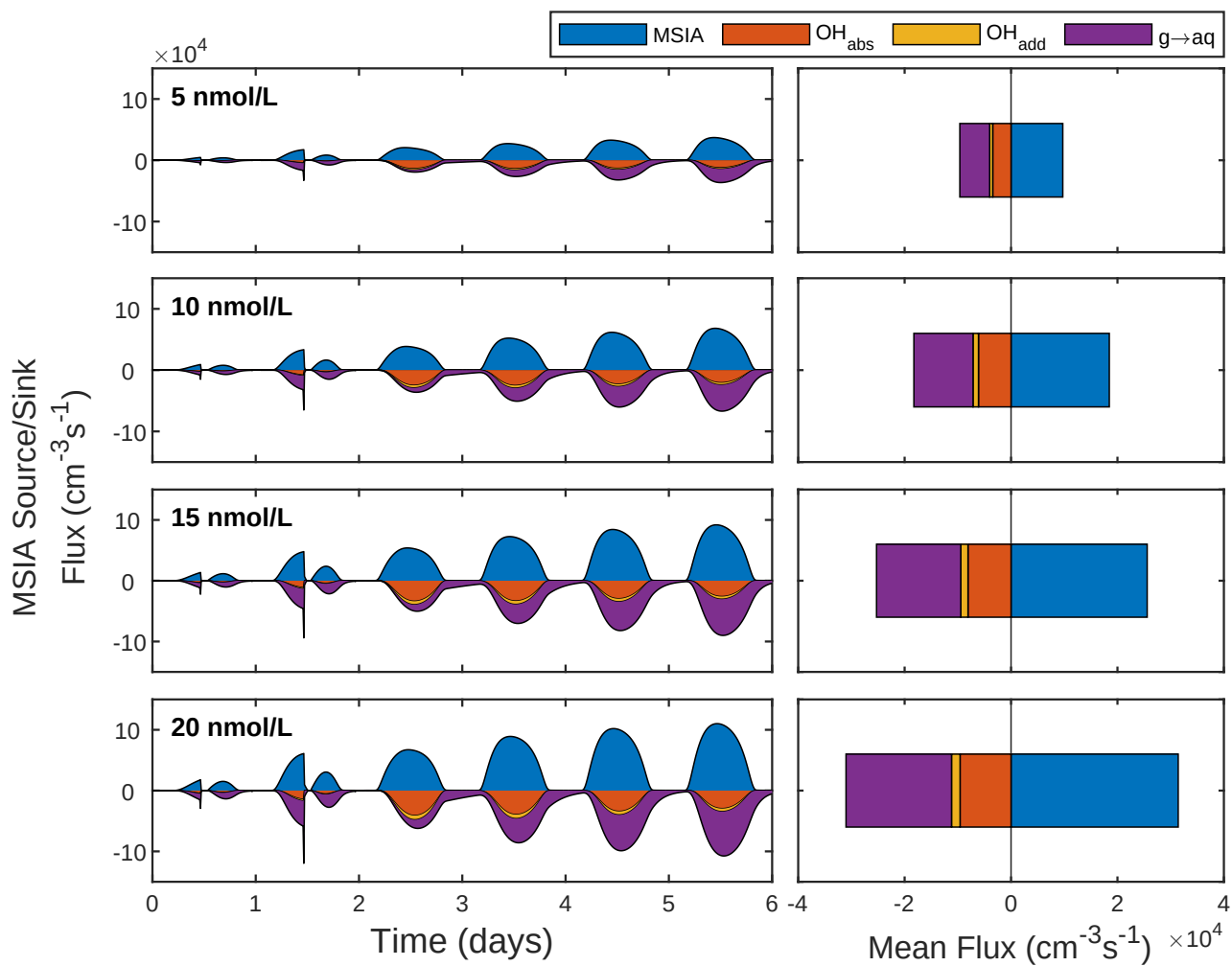


Figure S60. MSIA source/sink flux from DMSO and via reaction with OH (abstraction), OH (addition) and gas-aqueous phase uptake at varying DMS sea surface concentrations ranging from 5 nM to 20 nM. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

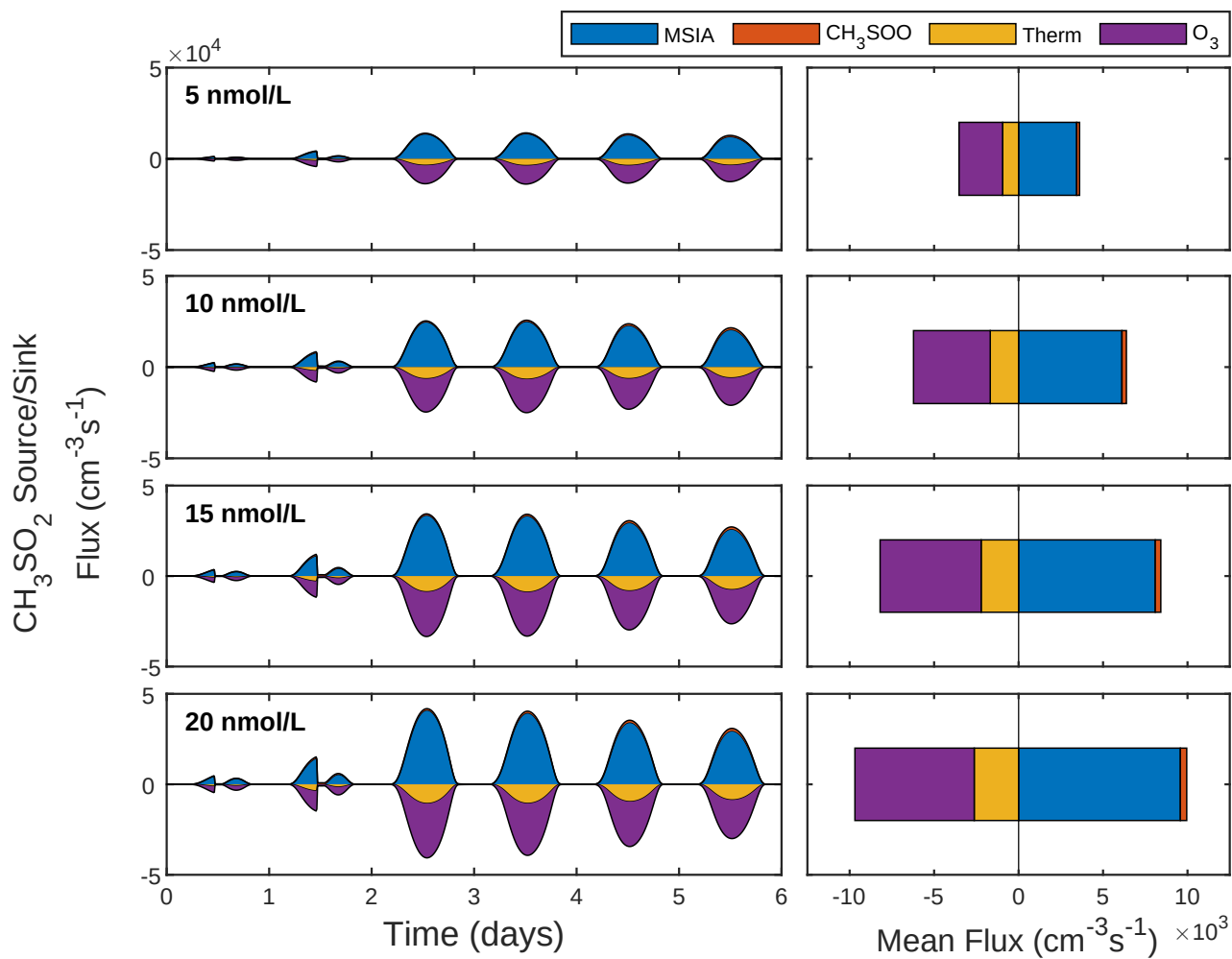


Figure S61. CH_3SO_2 source/sink flux from MSIA, CH_3SOO and via thermal decomposition and reaction with O_3 at varying DMS sea surface concentrations ranging from 5 nM to 20 nM. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

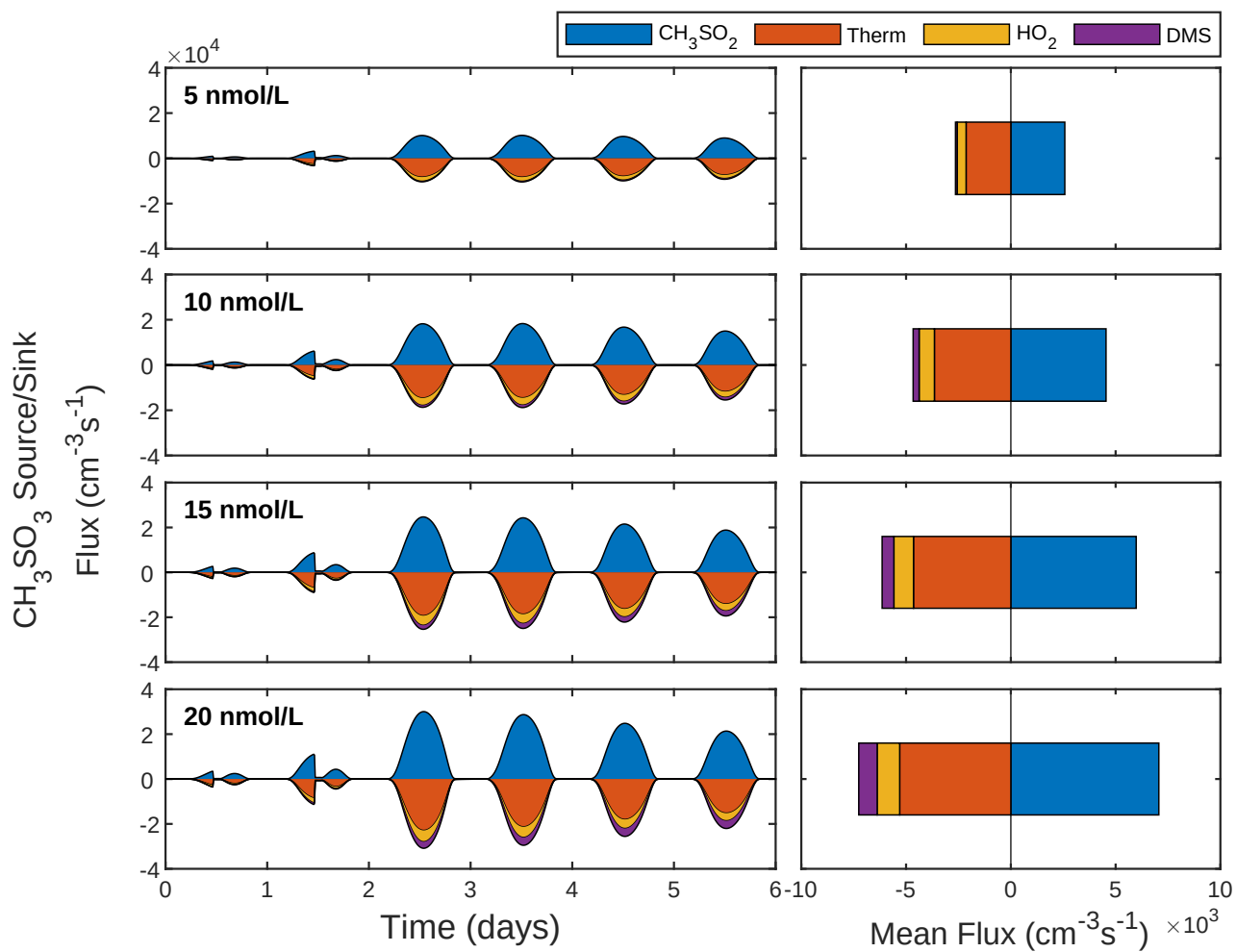


Figure S62. CH_3SO_3 source/sink flux from CH_3SO_2 , via thermal decomposition and reaction with HO_2 and DMS at varying DMS sea surface concentrations ranging from 5 nM to 20 nM. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

S11 Total seawater ammonia concentration sensitivity runs

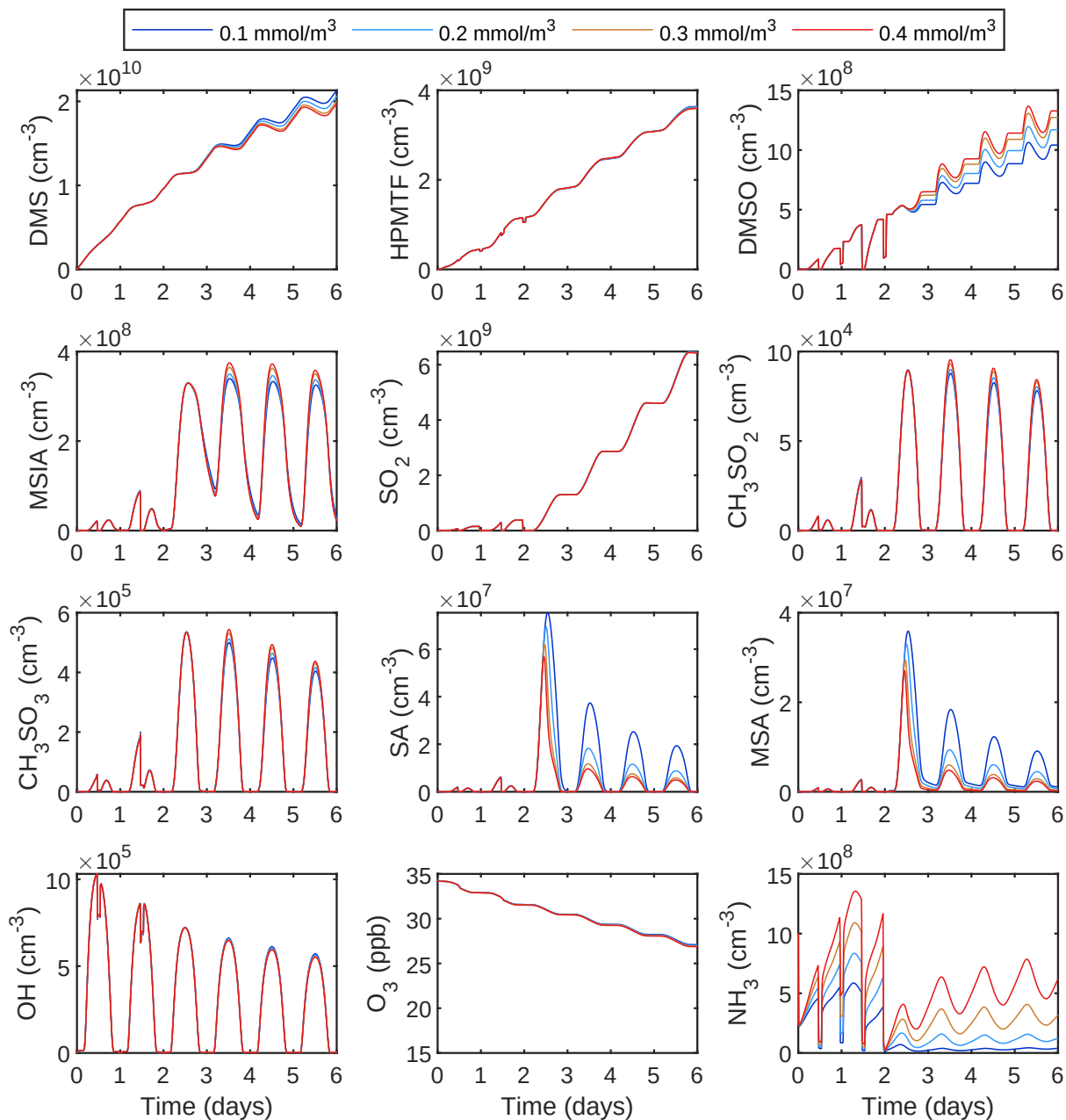


Figure S63. Concentrations of key gas-phase species at varying NH_x sea surface concentrations ranging from 0.1 mmol/m³ to 0.4 mmol/m³.

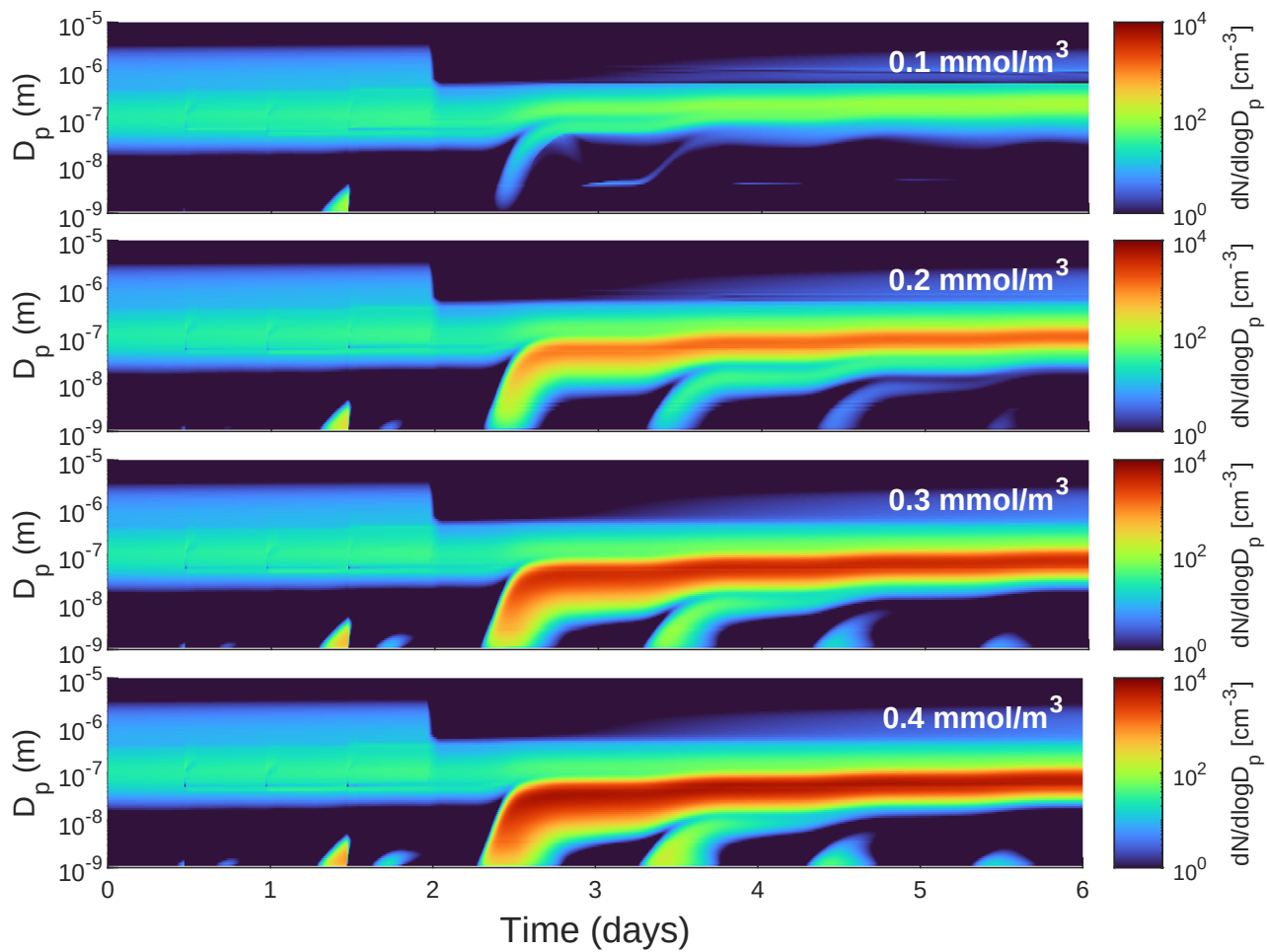


Figure S64. Aerosol particle number size distributions throughout the full simulation period at varying NH_x sea surface concentrations ranging from 0.1 mmol/m^3 to 0.4 mmol/m^3 .

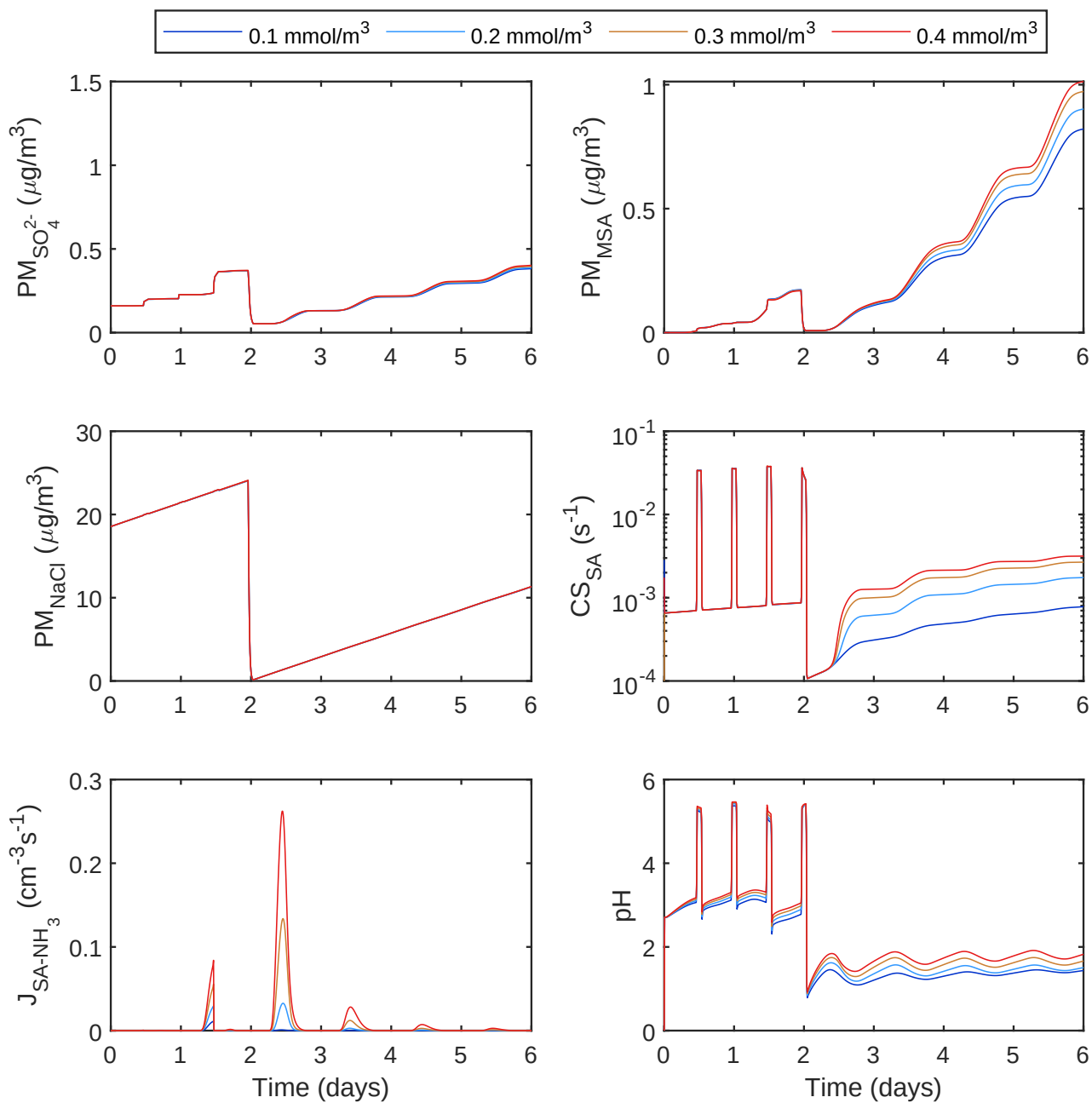


Figure S65. Total SO_4^{2-} , MSA and NaCl PM along with the SA condensation sink, SA- NH_3 driven nucleation rate and bulk pH at varying NH_x sea surface concentrations ranging from 0.1 mmol/m^3 to 0.4 mmol/m^3 .

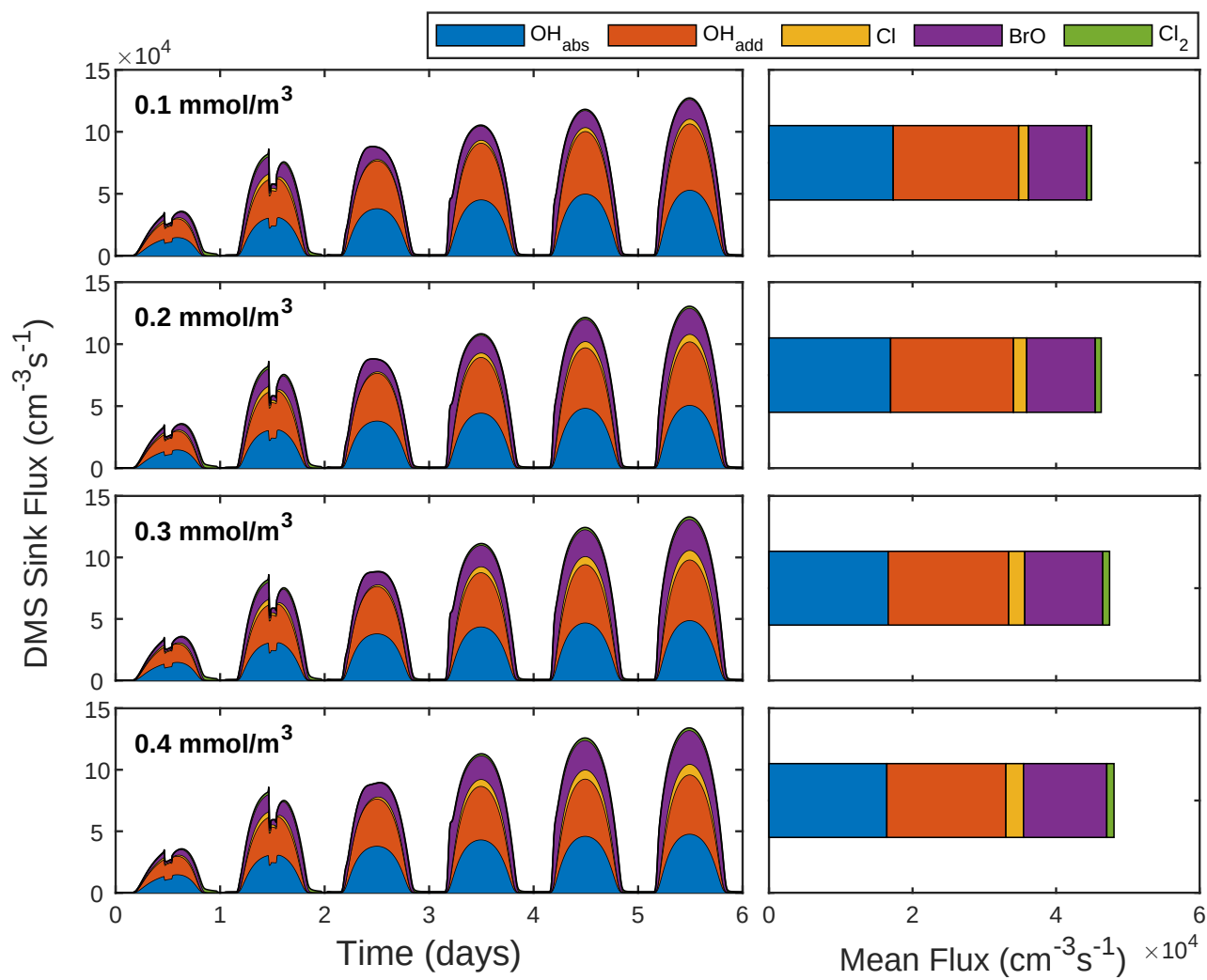


Figure S66. DMS sink flux driven by the reaction with OH (addition), OH (abstraction), Cl, BrO and Cl₂ at varying NH_x sea surface concentrations ranging from 0.1 mmol/m³ to 0.4 mmol/m³. Reactions that contribute < 1% of the total sink flux are not displayed in the figure.

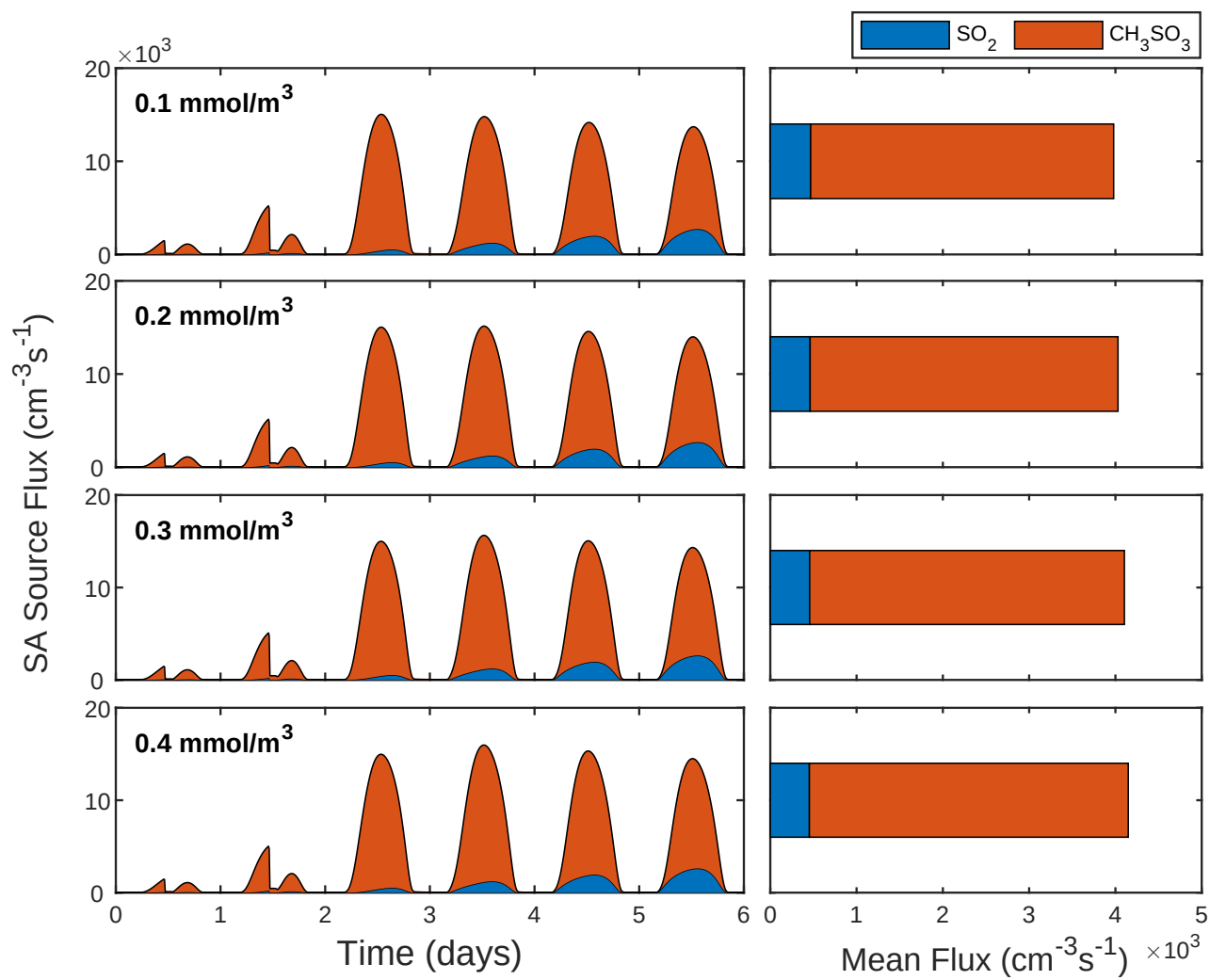


Figure S67. SA source flux from SO_2 and CH_3SO_3 at varying NH_x sea surface concentrations ranging from 0.1 mmol/m^3 to 0.4 mmol/m^3 .

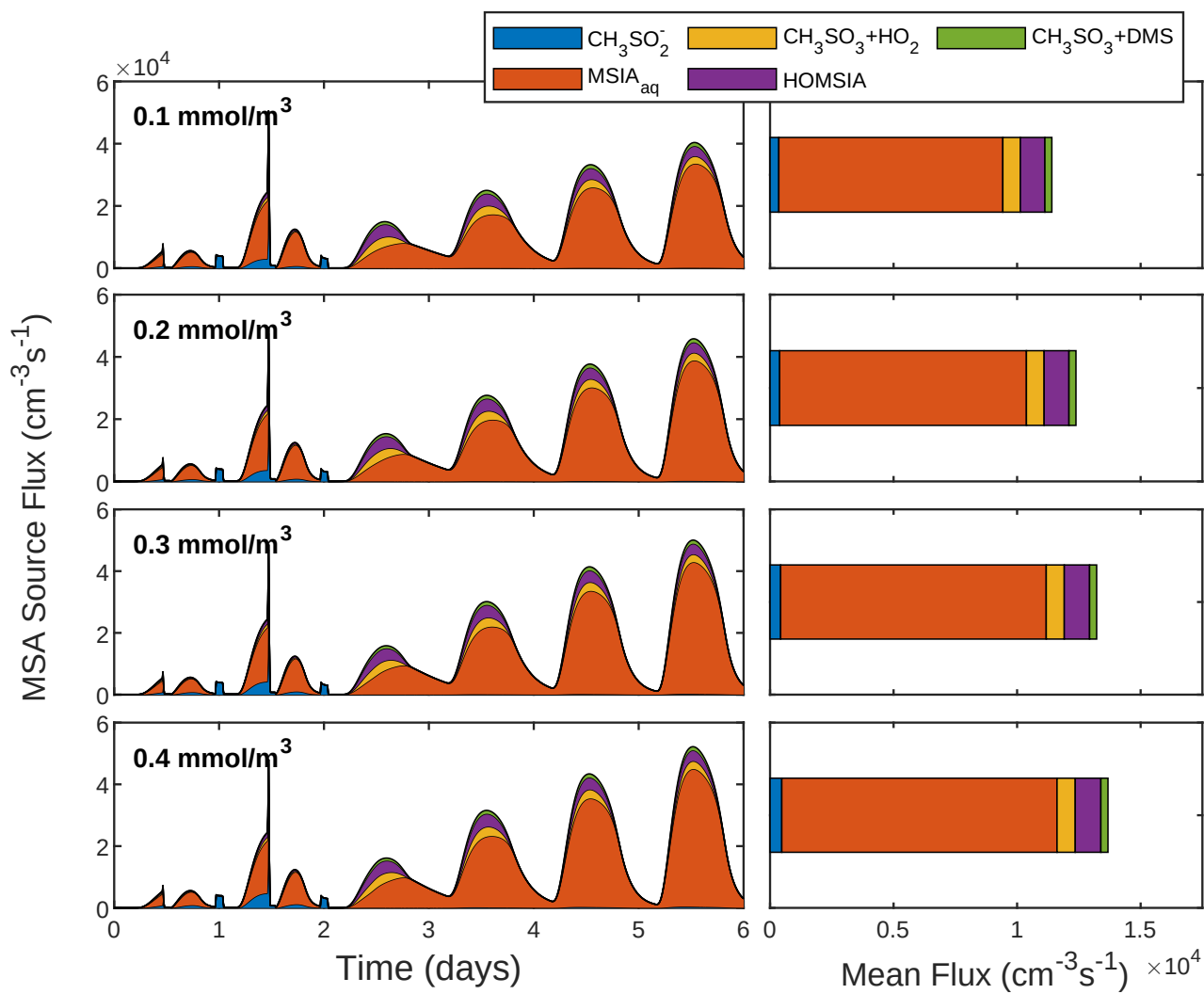


Figure S68. MSA source flux from CH₃SO₂⁻ and MSIA_{aq} in the aqueous-phase in addition to CH₃SO₃ via HO₂, CH₃SO₃ via DMS and HOMSA in the gas-phase at varying NH_x sea surface concentrations ranging from 0.1 mmol/m³ to 0.4 mmol/m³.

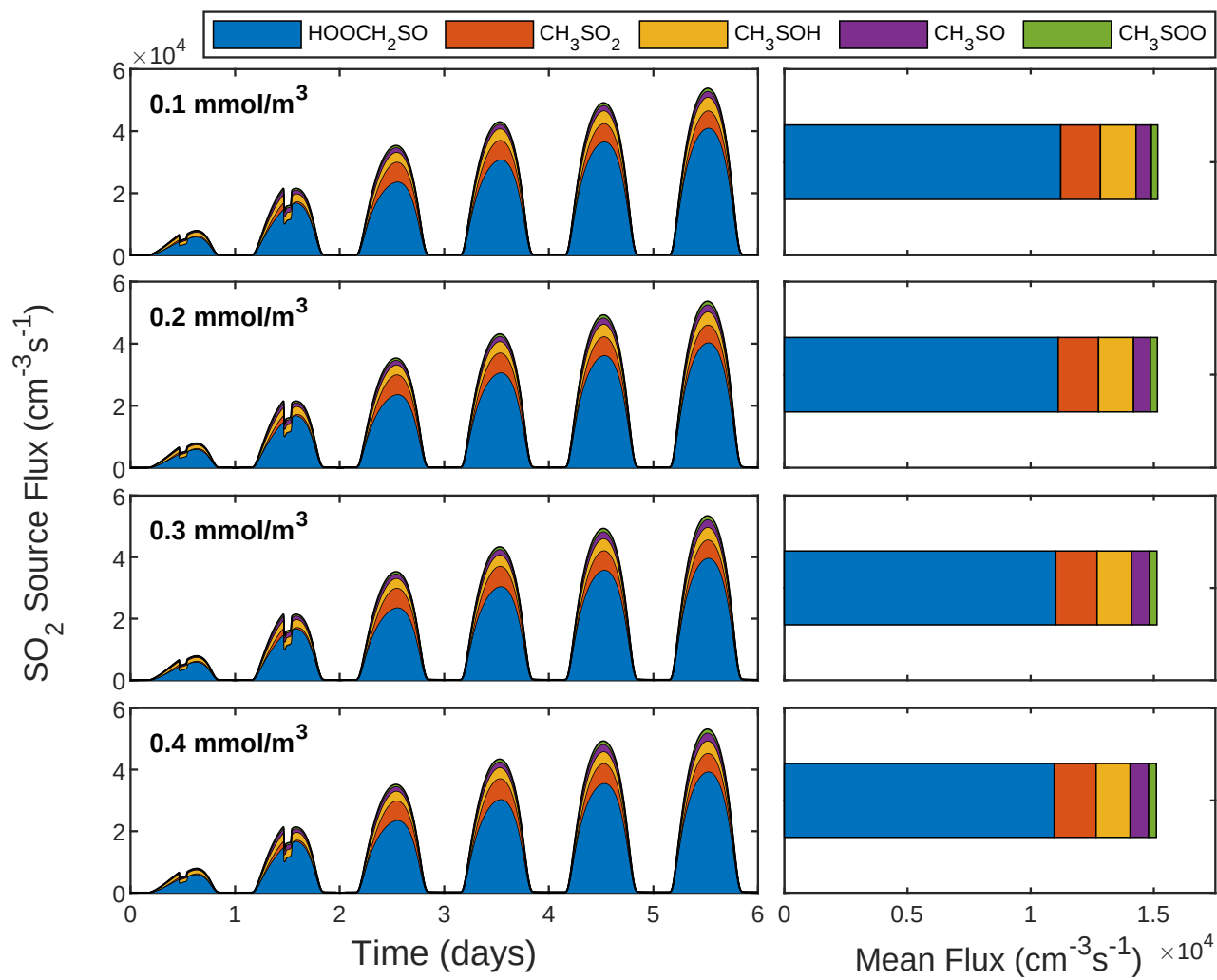


Figure S69. SO₂ source flux from HOOCH₂SO, CH₃SO₂, CH₃SOH, CH₃SO and CH₃SOO at varying NH_x sea surface concentrations ranging from 0.1 mmol/m³ to 0.4 mmol/m³. Reactions that contribute < 1% of the total source flux are not displayed in the figure.

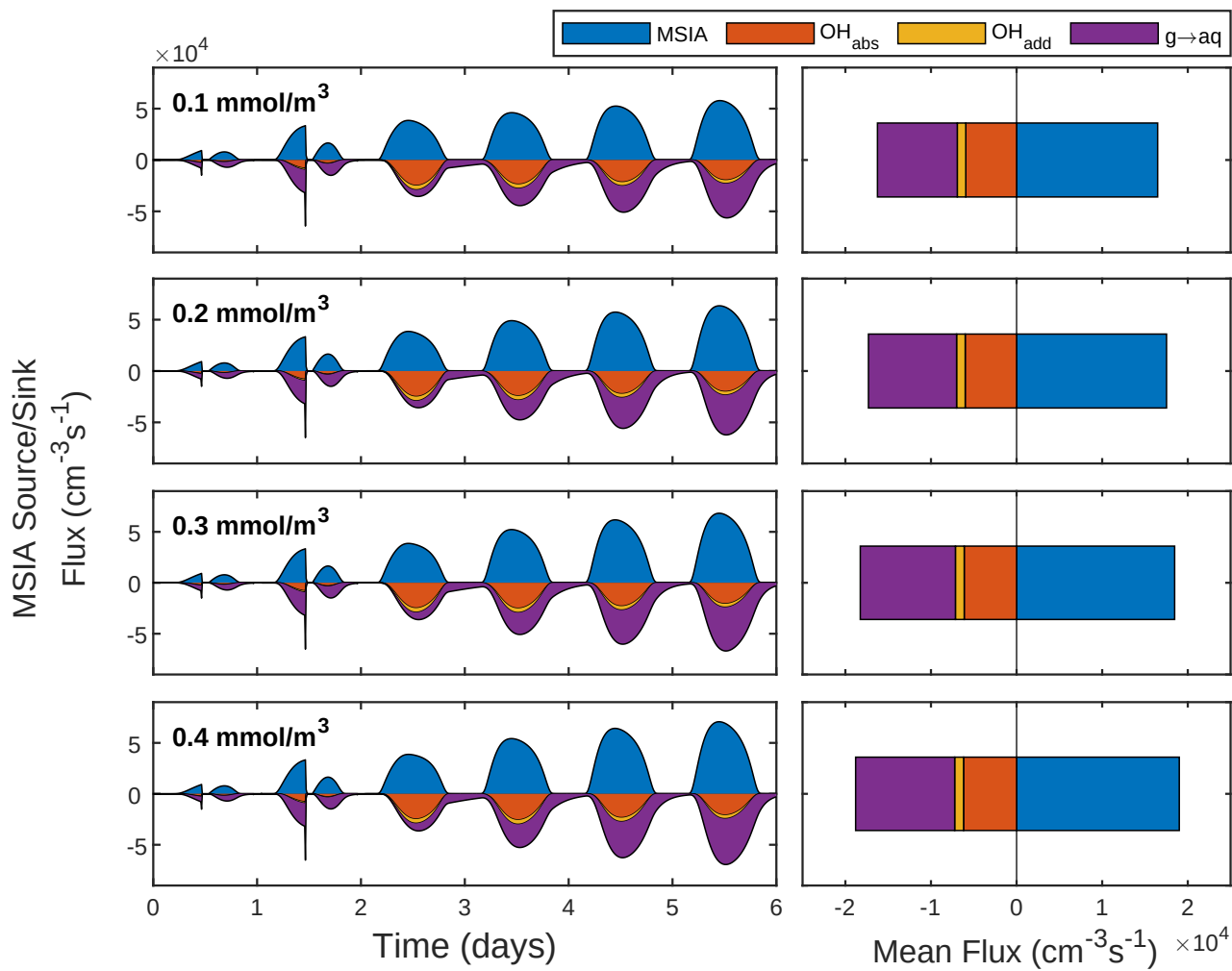


Figure S70. MSIA source/sink flux from DMSO and via reaction with OH (abstraction), OH (addition) and gas-aqueous phase uptake at varying NH_x sea surface concentrations ranging from 0.1 mmol/m^3 to 0.4 mmol/m^3 . Reactions that contribute $< 1\%$ of the total source/sink flux are not displayed in the figure.

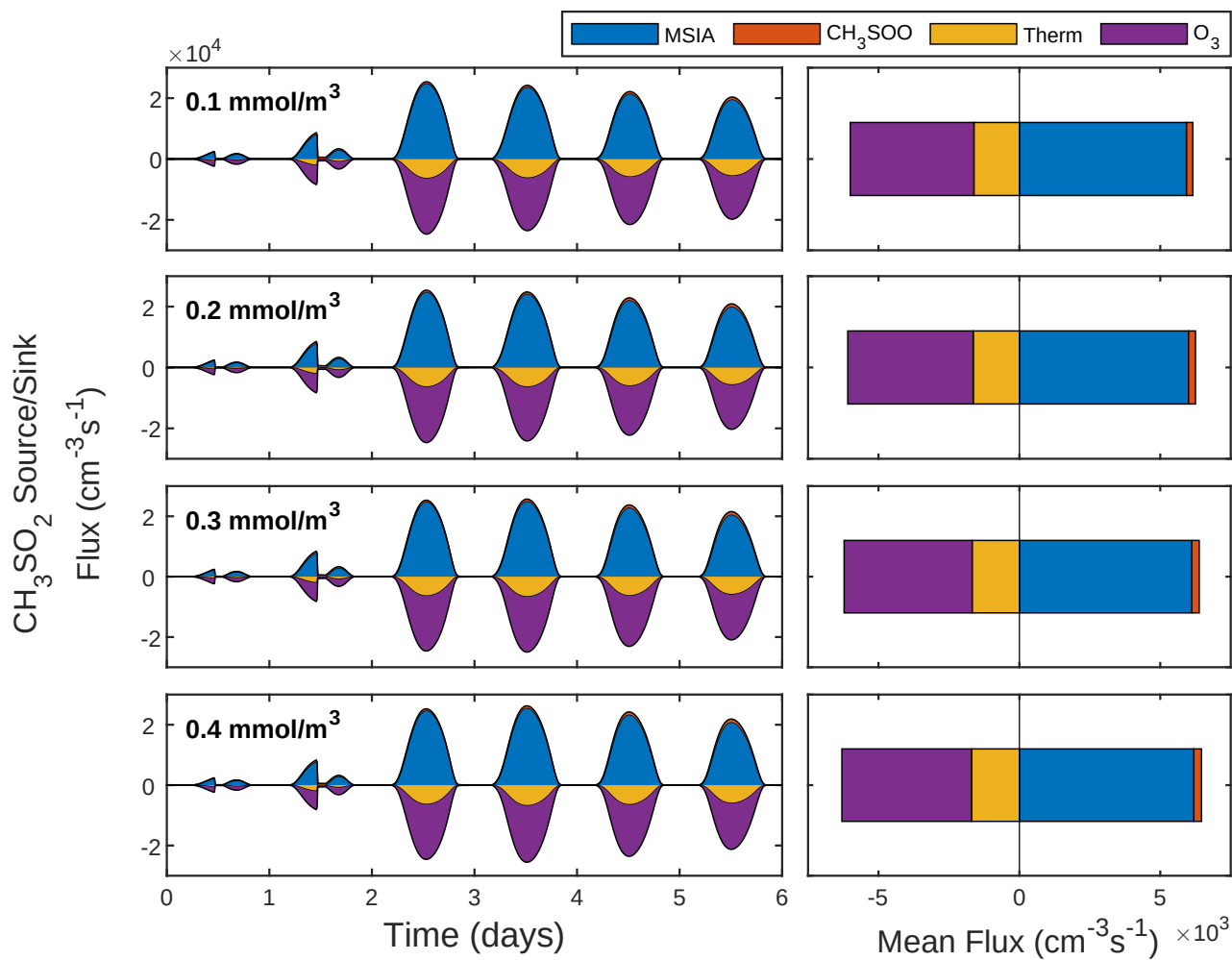


Figure S71. CH_3SO_2 source/sink flux from MSIA, CH_3SOO and via thermal decomposition and reaction with O_3 at varying NH_x sea surface concentrations ranging from 0.1 mmol/m^3 to 0.4 mmol/m^3 . Reactions that contribute $< 1\%$ of the total source/sink flux are not displayed in the figure.

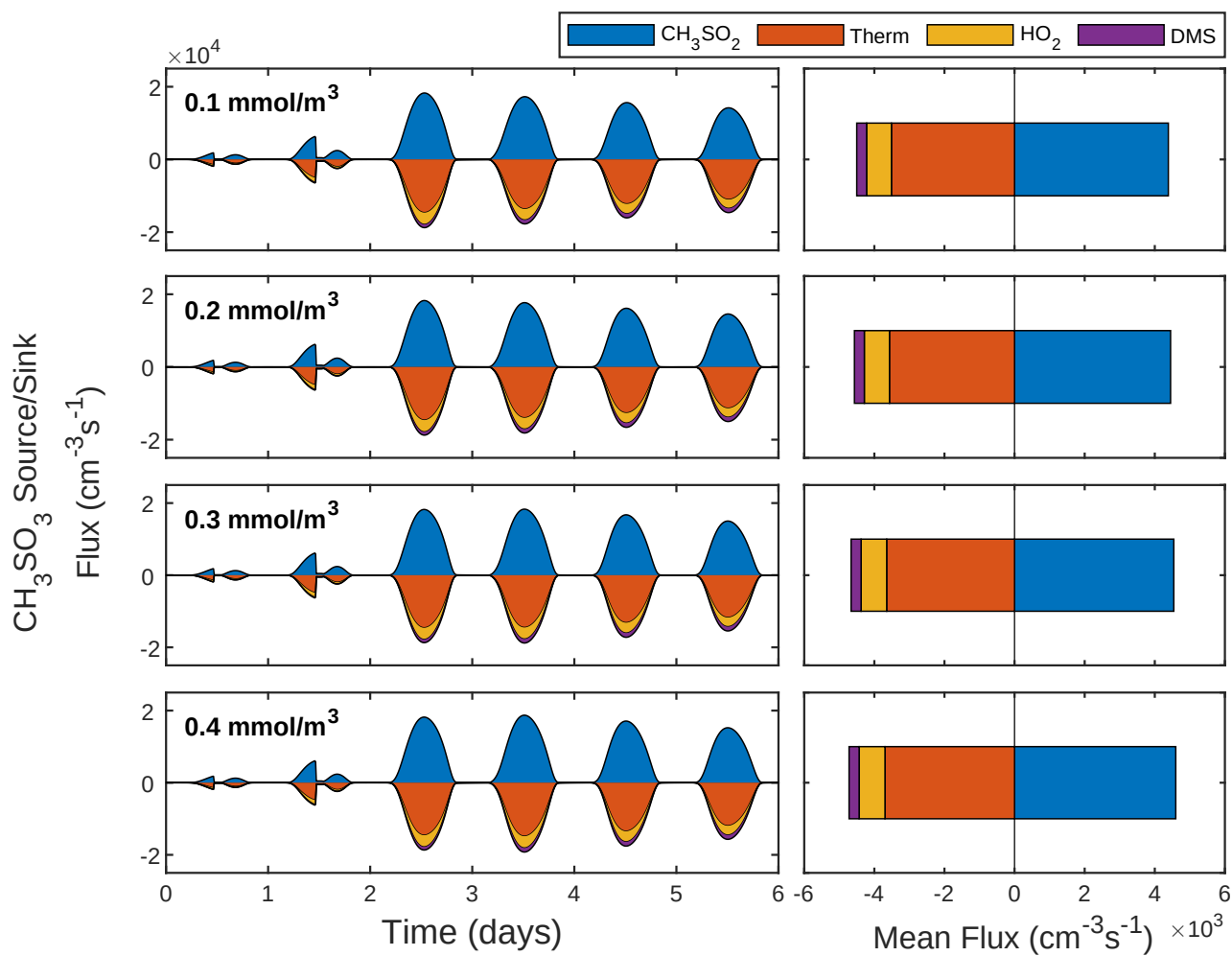


Figure S72. CH_3SO_3 source/sink flux from CH_3SO_2 , via thermal decomposition and reaction with HO_2 and DMS at varying NH_x sea surface concentrations ranging from 0.1 mmol/m^3 to 0.4 mmol/m^3 . Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

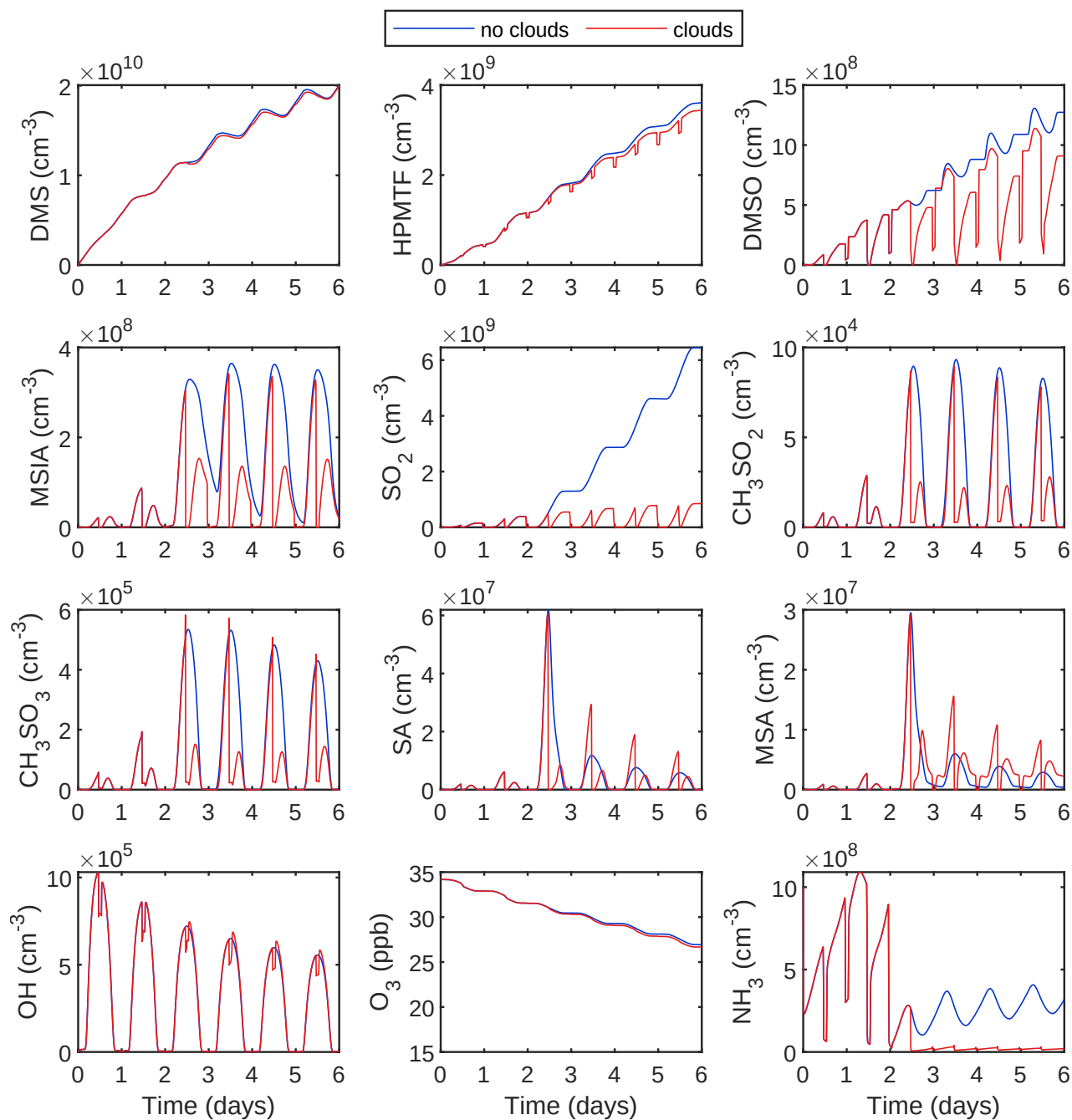


Figure S73. Concentrations of key gas-phase species during conditions with and without clouds.

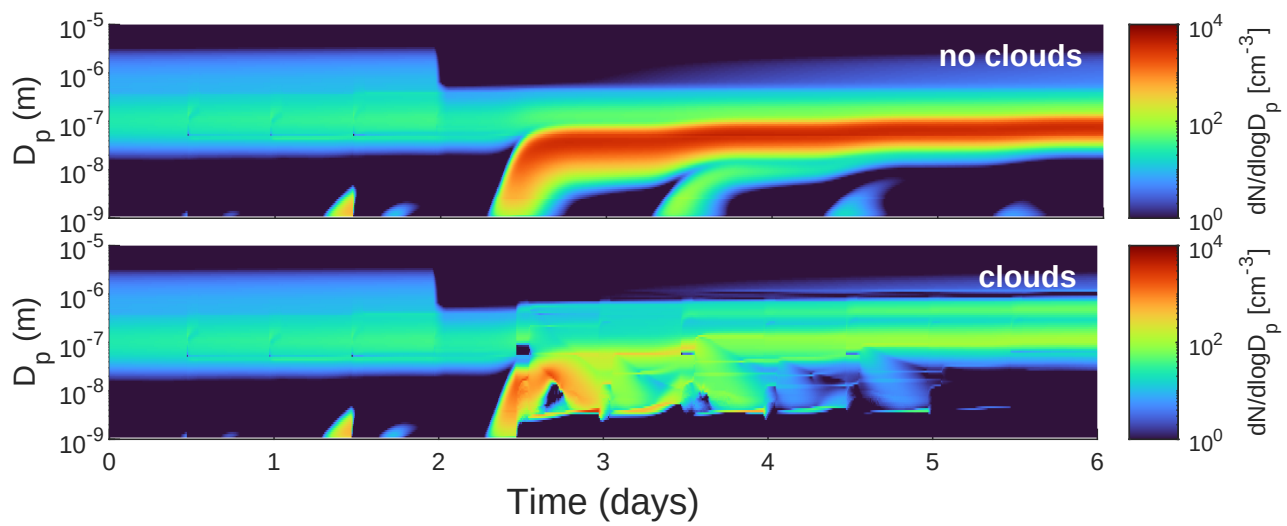


Figure S74. Aerosol particle number size distributions throughout the full simulation period during conditions with and without clouds.

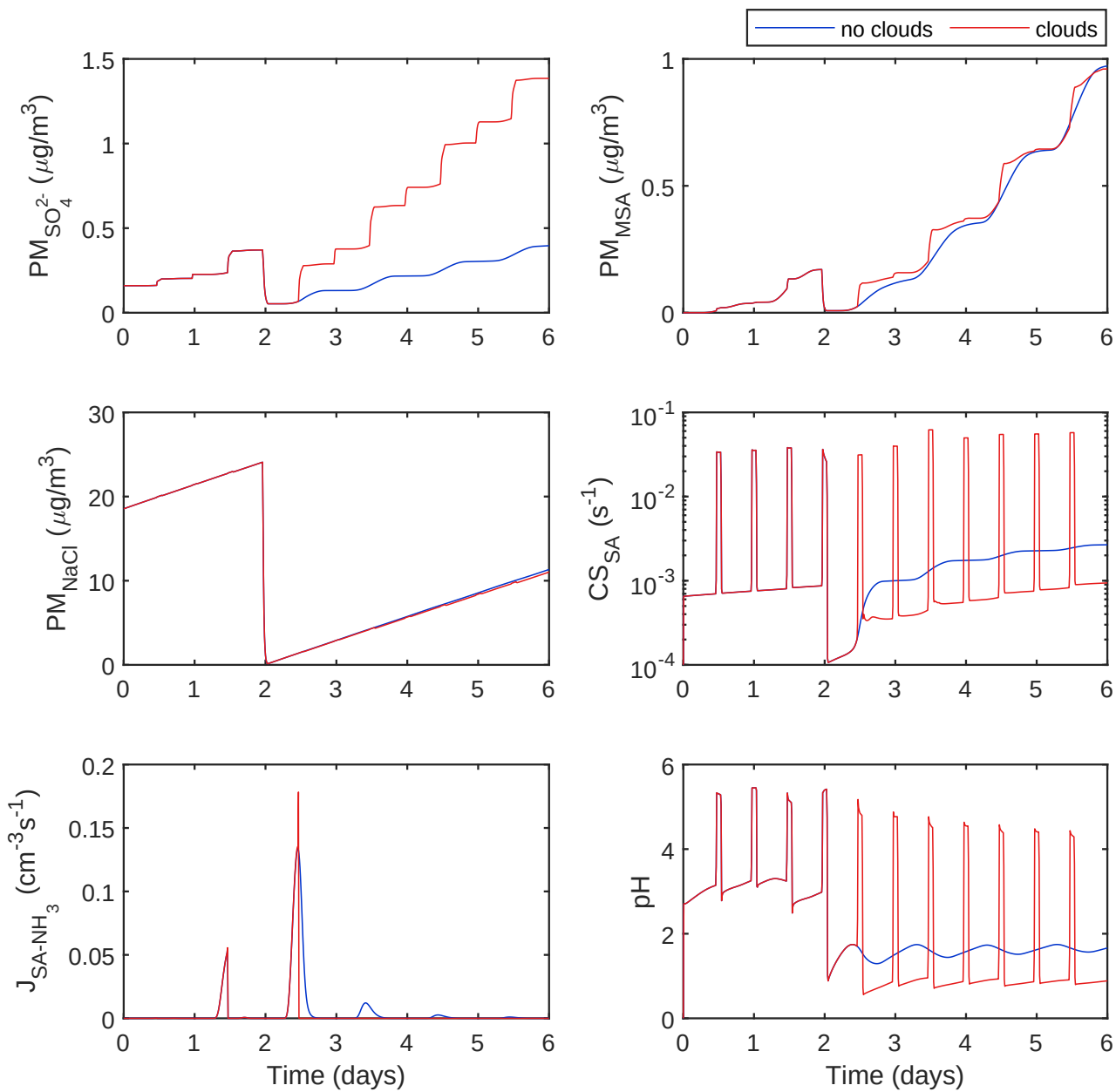


Figure S75. Total SO_4^{2-} , MSA and NaCl PM along with the SA condensation sink, SA- NH_3 driven nucleation rate and bulk pH during conditions with and without clouds.

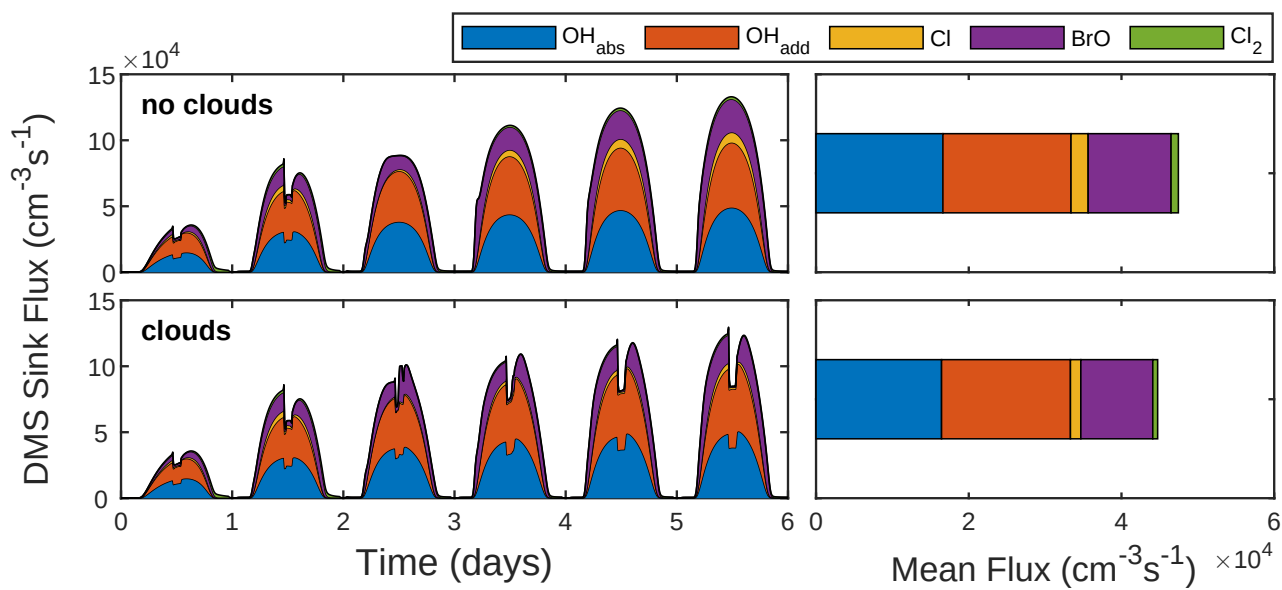


Figure S76. DMS sink flux driven by the reaction with OH (addition), OH (abstraction), Cl, BrO and Cl₂ during conditions with and without clouds. Reactions that contribute < 1% of the total sink flux are not displayed in the figure.

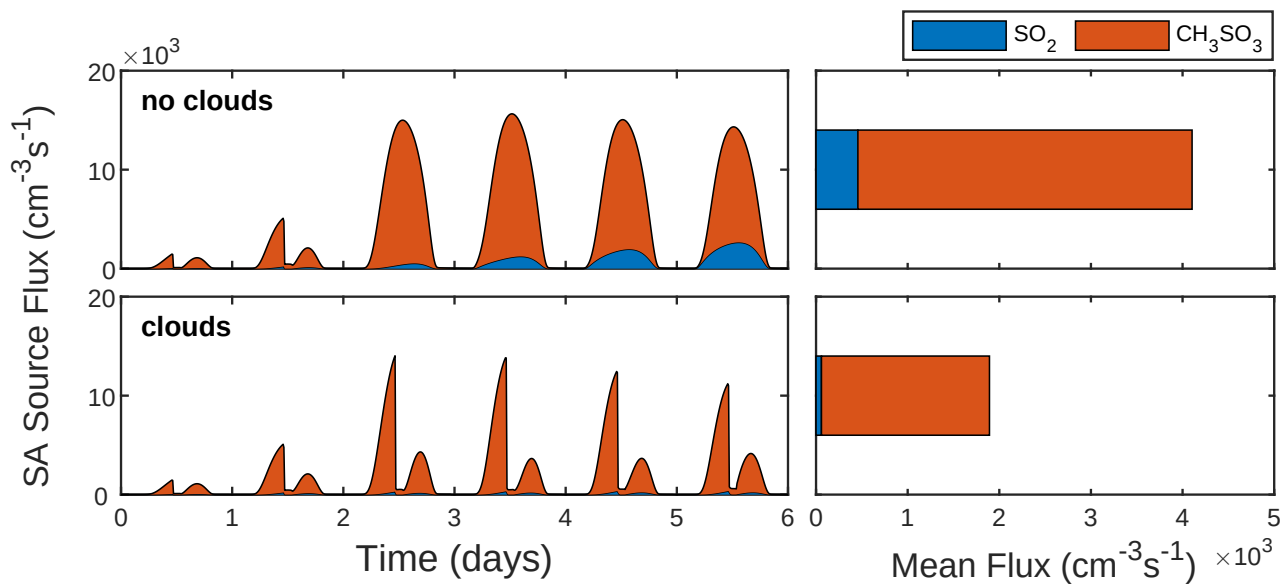


Figure S77. SA source flux from SO₂ and CH₃SO₃ during conditions with and without clouds.

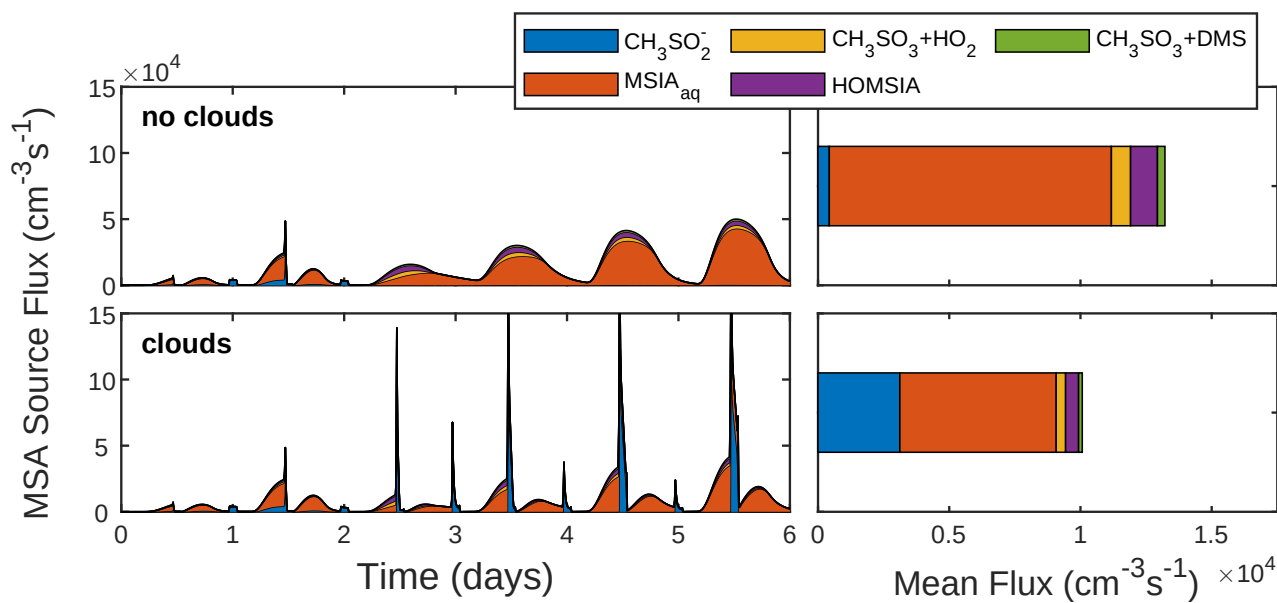


Figure S78. MSA source flux from CH_3SO_2^- and MSIA_{aq} in the aqueous-phase in addition to CH_3SO_3 via HO_2 , CH_3SO_3 via DMS and HOMSIA in the gas-phase during conditions with and without clouds.

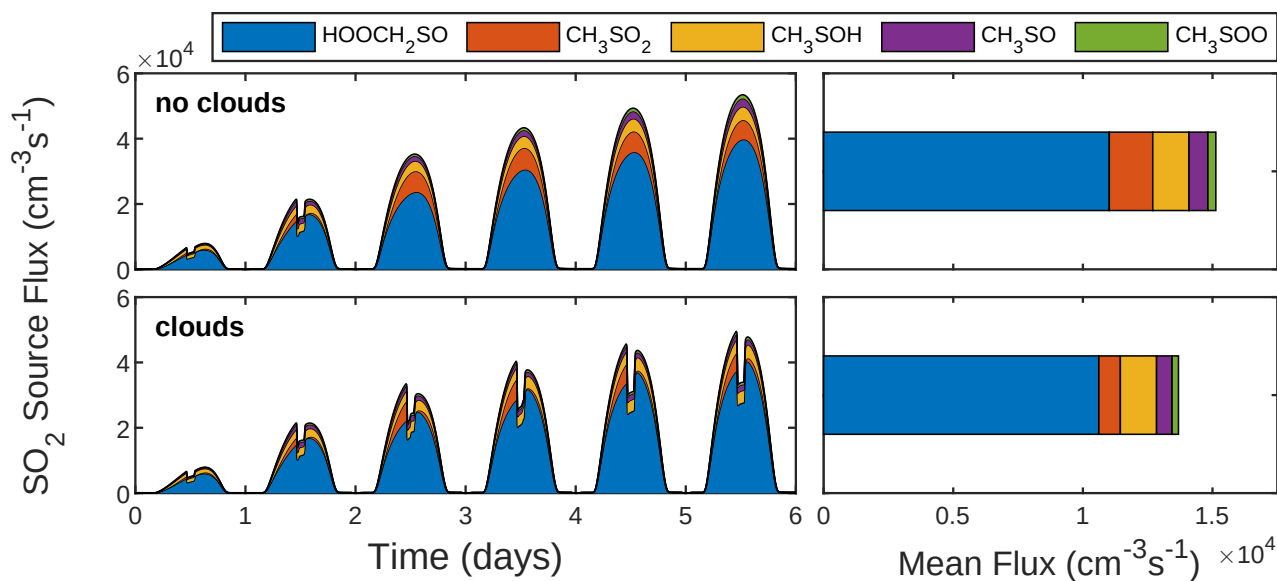


Figure S79. SO_2 source flux from HOOCH_2SO , CH_3SO_2 , CH_3SOH , CH_3SO and CH_3SOO during conditions with and without clouds. Reactions that contribute $< 1\%$ of the total source flux are not displayed in the figure.

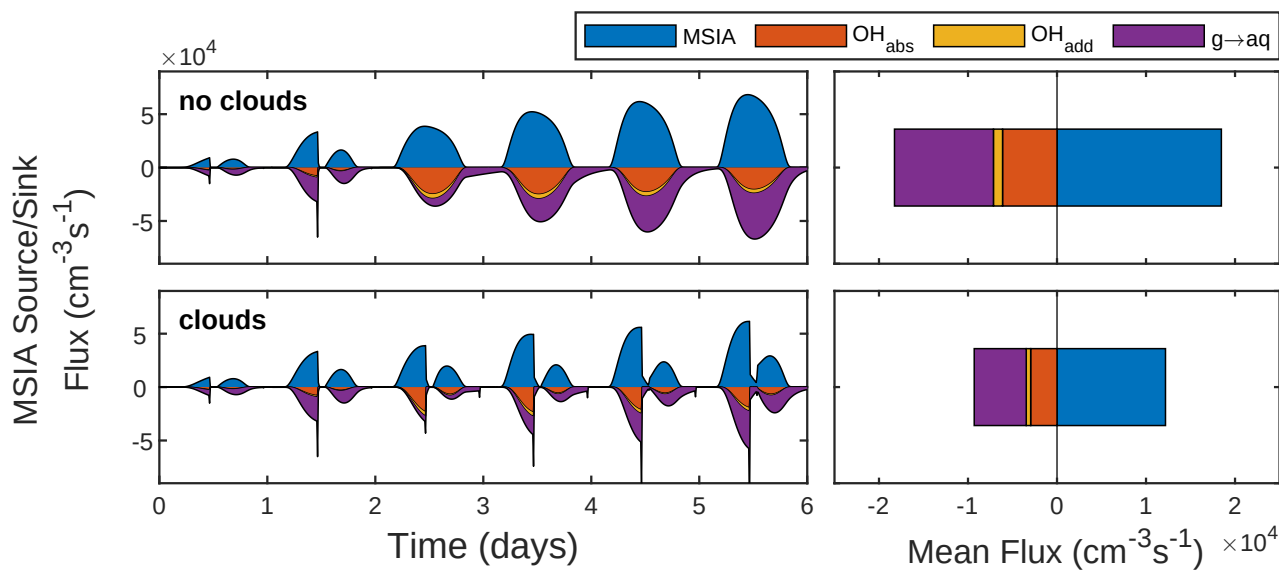


Figure S80. MSIA source/sink flux from DMSO and via reaction with OH (abstraction), OH (addition) and gas-aqueous phase uptake during conditions with and without clouds. Reactions that contribute $< 1\%$ of the total source/sink flux are not displayed in the figure.

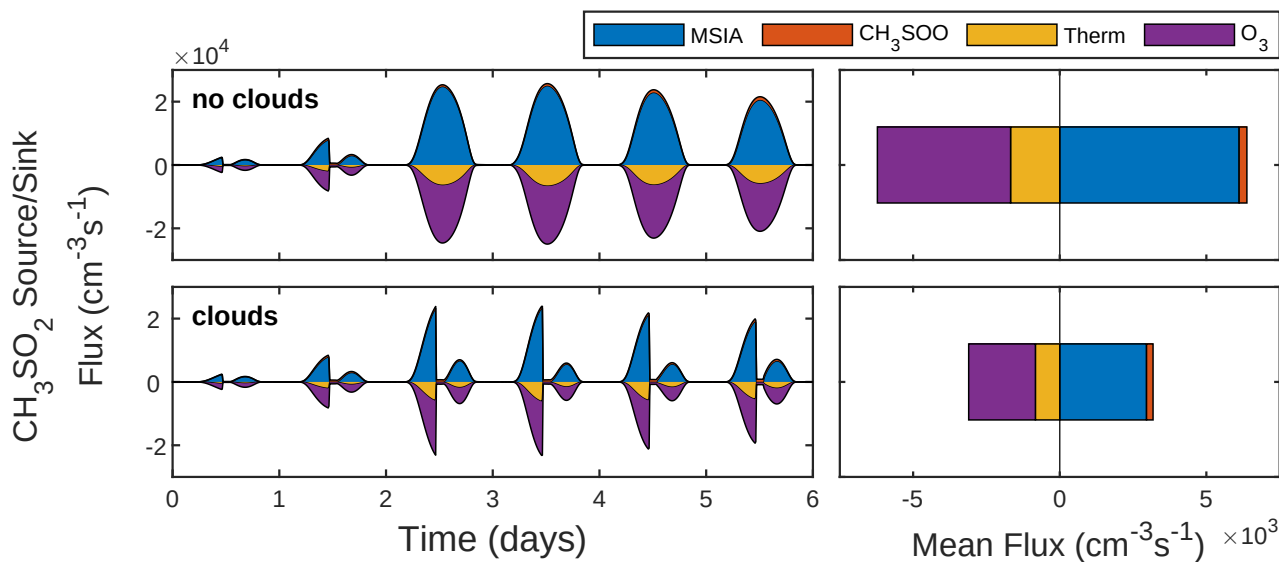


Figure S81. CH_3SO_2 source/sink flux from MSIA, CH_3SOO and via thermal decomposition and reaction with O_3 during conditions with and without clouds. Reactions that contribute $< 1\%$ of the total source/sink flux are not displayed in the figure.

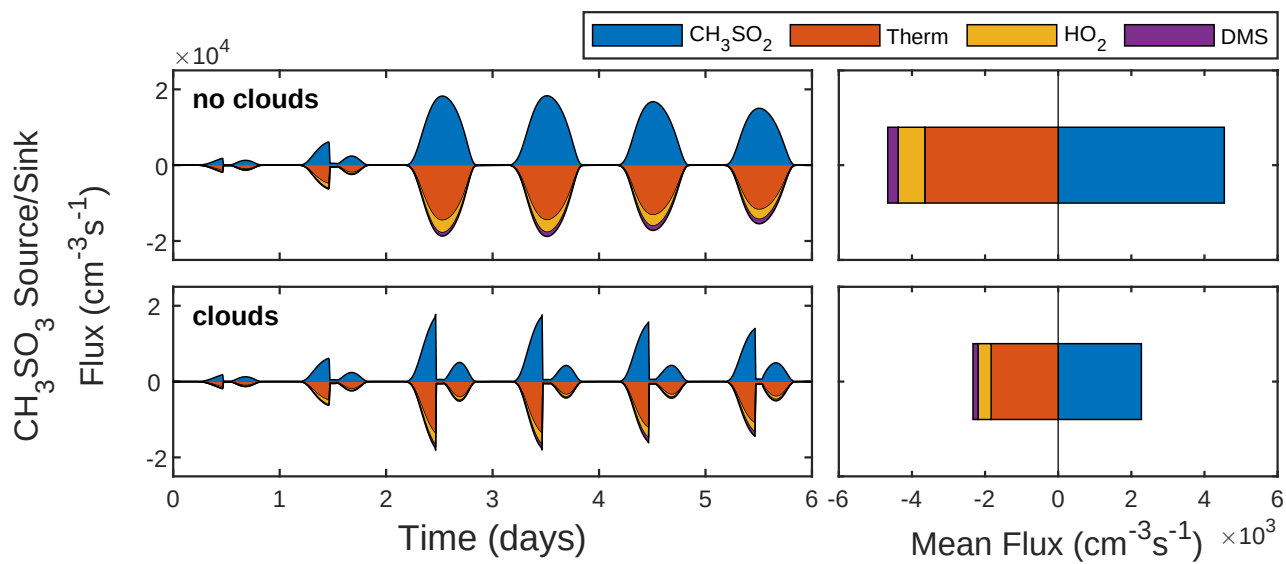


Figure S82. CH_3SO_3 source/sink flux from CH_3SO_2 , via thermal decomposition and reaction with HO_2 and DMS during conditions with and without clouds. Reactions that contribute $< 1\%$ of the total source/sink flux are not displayed in the figure.

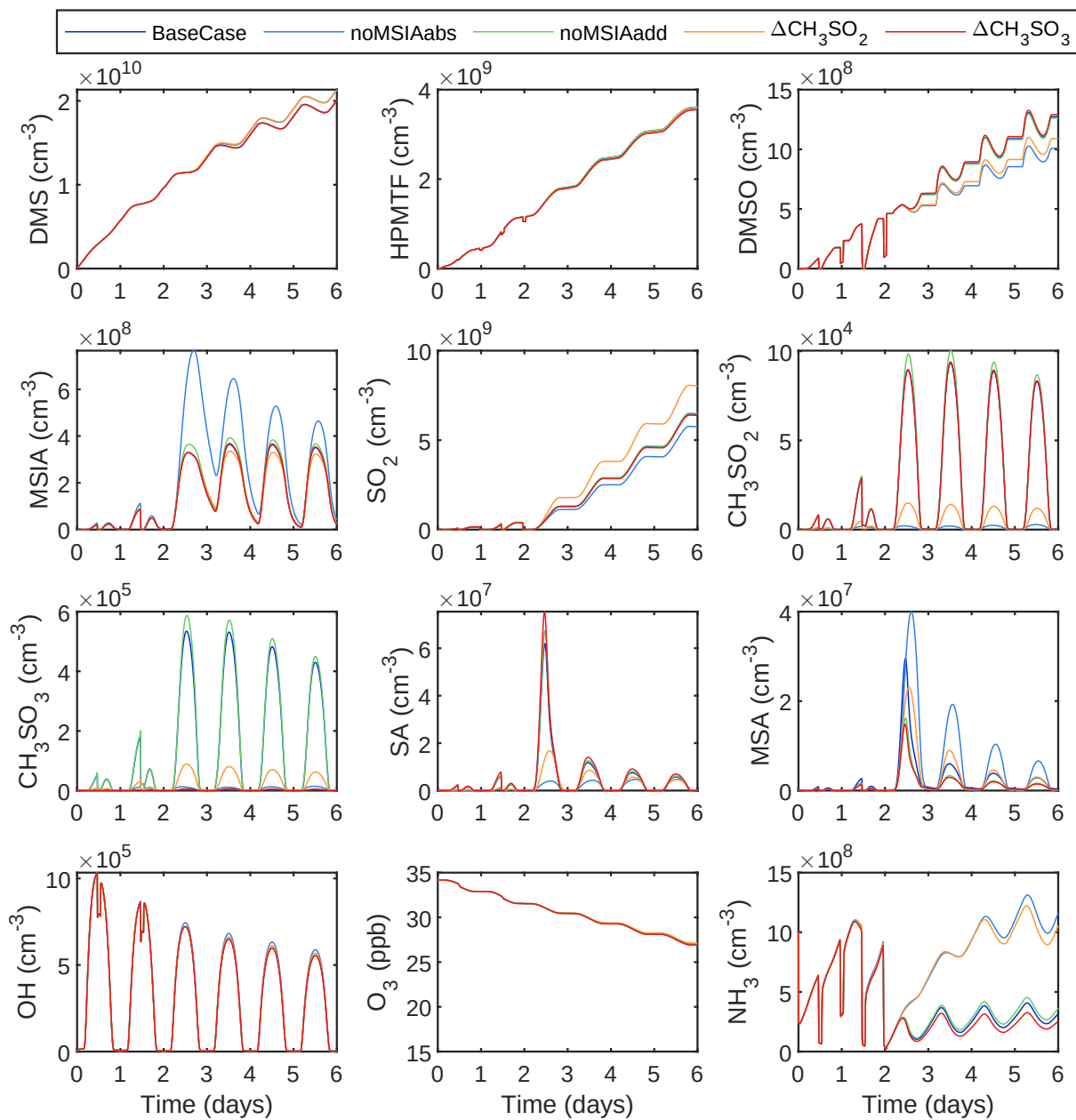


Figure S83. Concentrations of key gas-phase species for the BaseCase simulation and the noMSIAabs, noMSIAadd, $\Delta\text{CH}_3\text{SO}_2$ and $\Delta\text{CH}_3\text{SO}_3$ sensitivity runs.

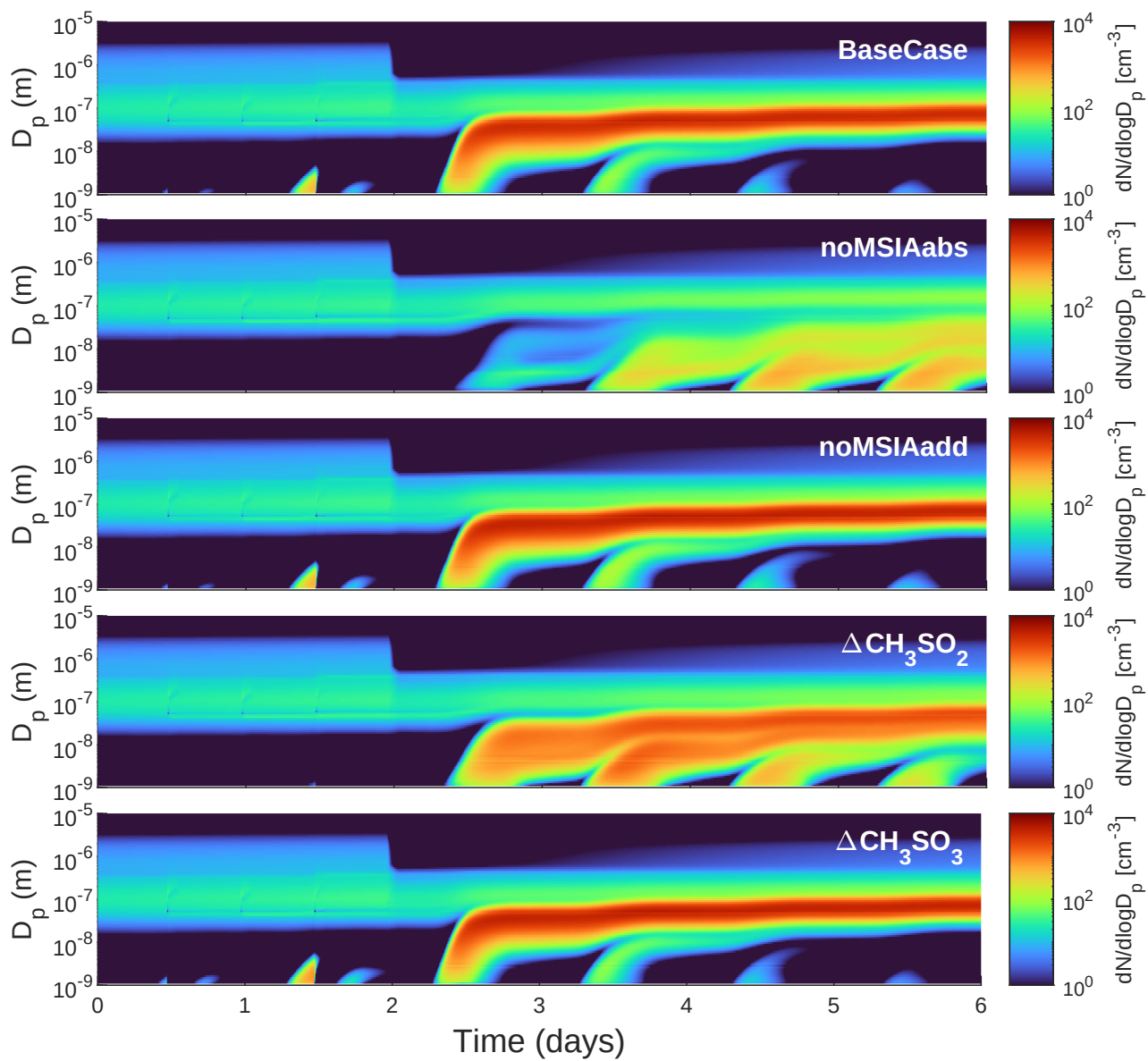


Figure S84. Aerosol particle number size distributions throughout the full simulation period for the BaseCase simulation and the noMSIAabs, noMSIAadd, $\Delta\text{CH}_3\text{SO}_2$ and $\Delta\text{CH}_3\text{SO}_3$ sensitivity runs.

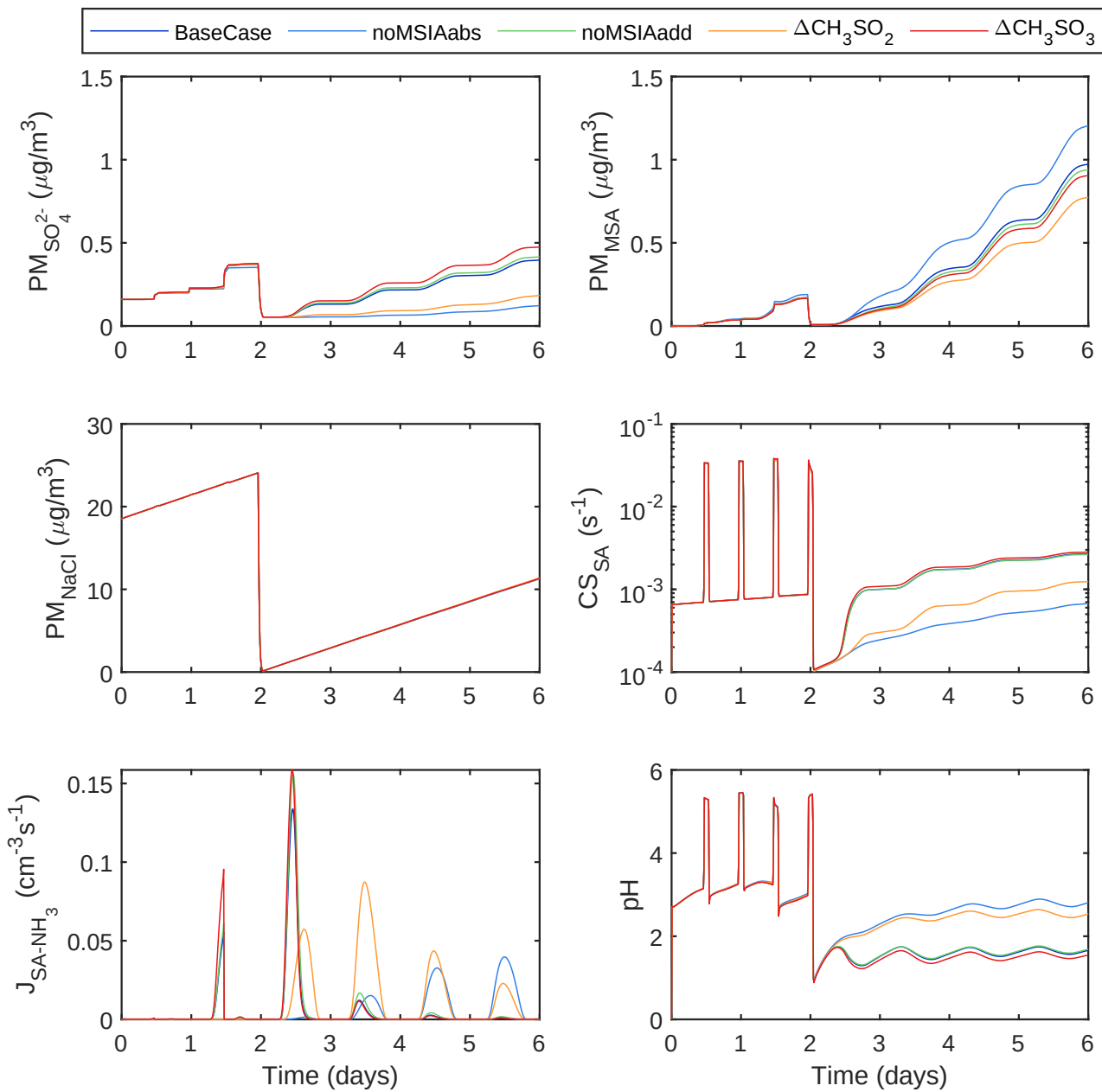


Figure S85. Total SO_4^{2-} , MSA and NaCl PM along with the SA condensation sink, SA- NH_3 driven nucleation rate and bulk pH for the BaseCase simulation and the noMSIAabs, noMSIAadd, $\Delta\text{CH}_3\text{SO}_2$ and $\Delta\text{CH}_3\text{SO}_3$ sensitivity runs.

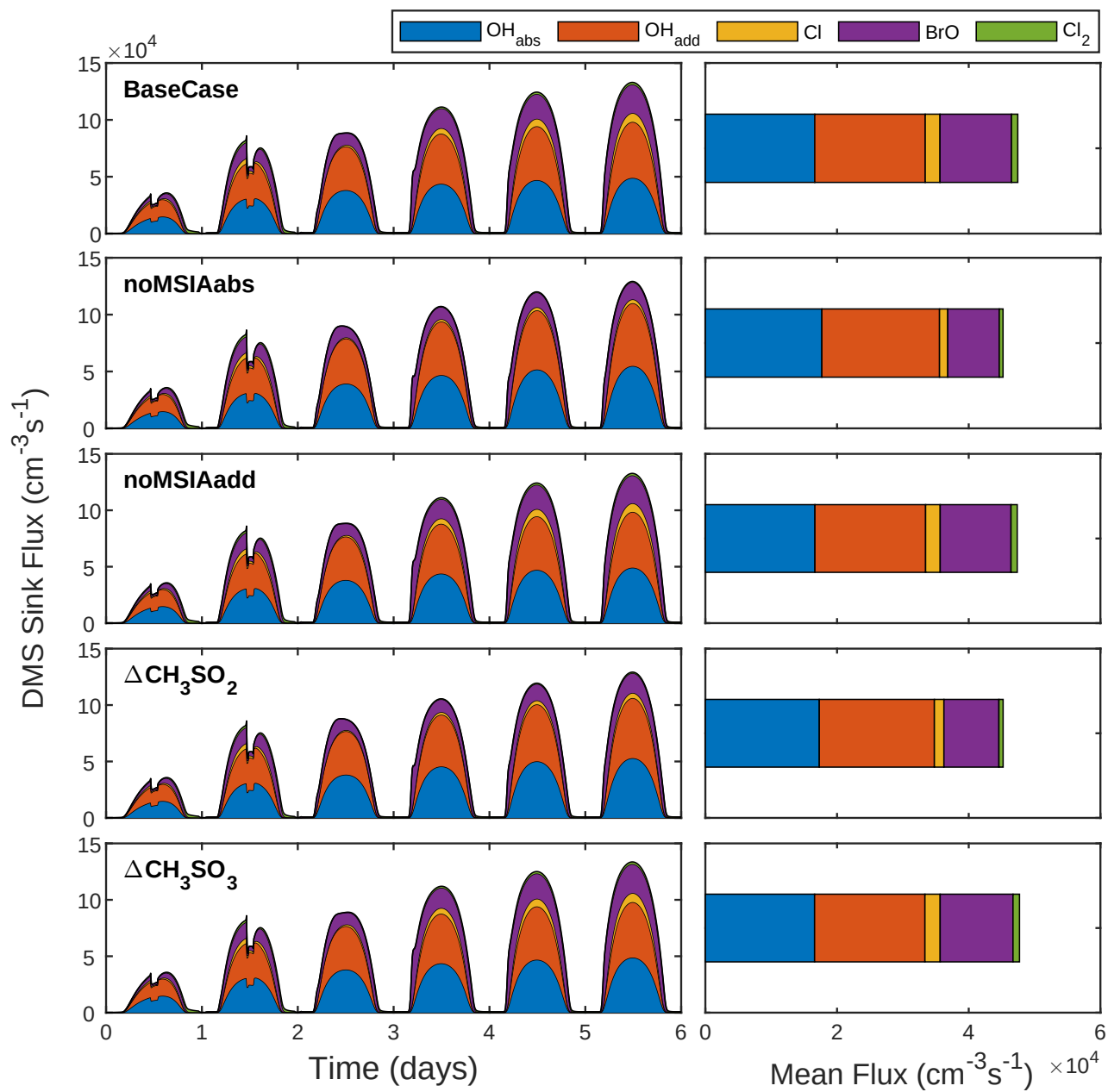


Figure S86. DMS sink flux driven by the reaction with OH (addition), OH (abstraction), Cl, BrO and Cl₂ for the BaseCase simulation and the noMSIAabs, noMSIAadd, $\Delta\text{CH}_3\text{SO}_2$ and $\Delta\text{CH}_3\text{SO}_3$ sensitivity runs. Reactions that contribute < 1% of the total sink flux are not displayed in the figure.

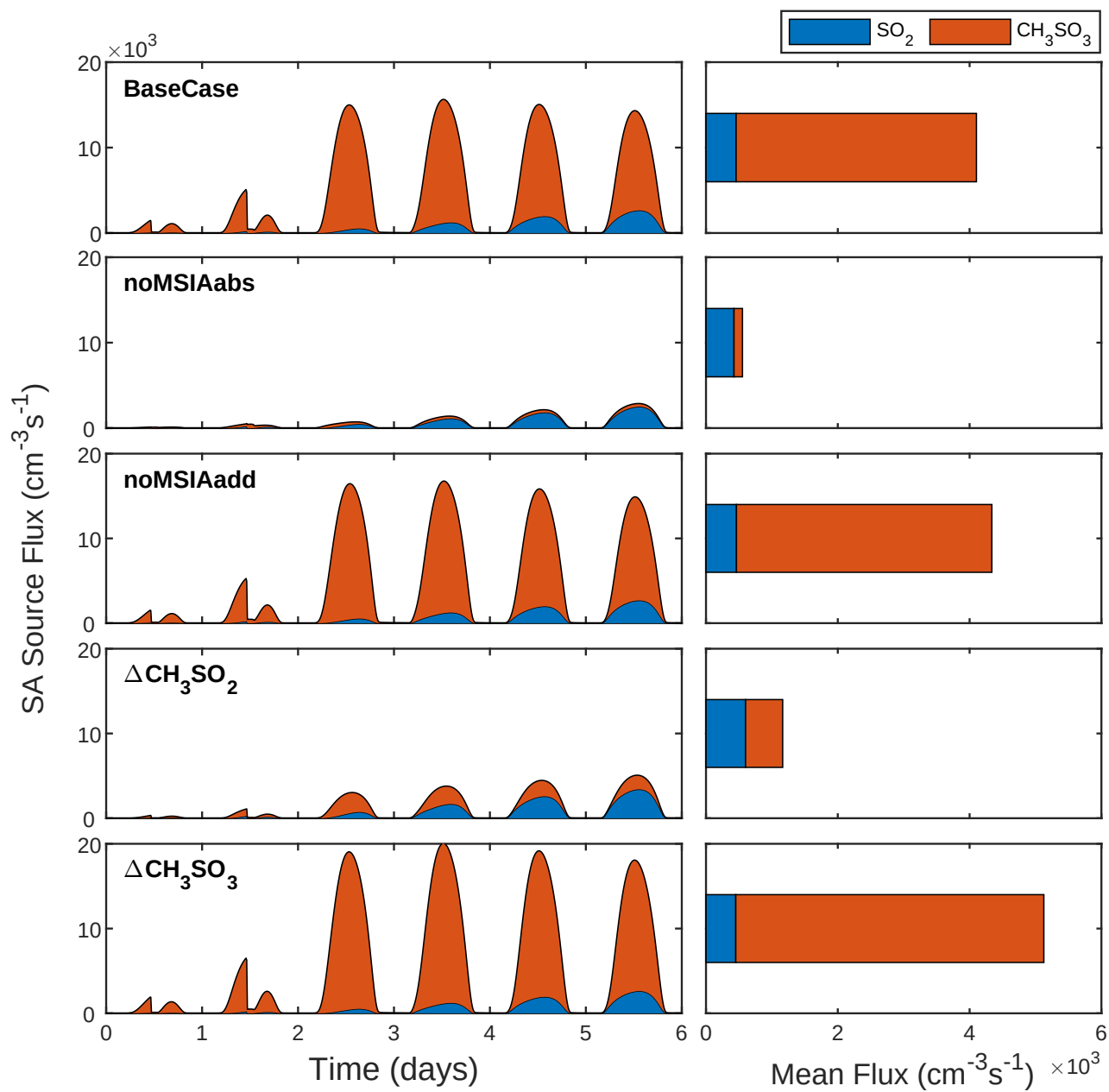


Figure S87. SA source flux from SO_2 and CH_3SO_3 for the BaseCase simulation and the noMSIAabs, noMSIAadd, $\Delta\text{CH}_3\text{SO}_2$ and $\Delta\text{CH}_3\text{SO}_3$ sensitivity runs.

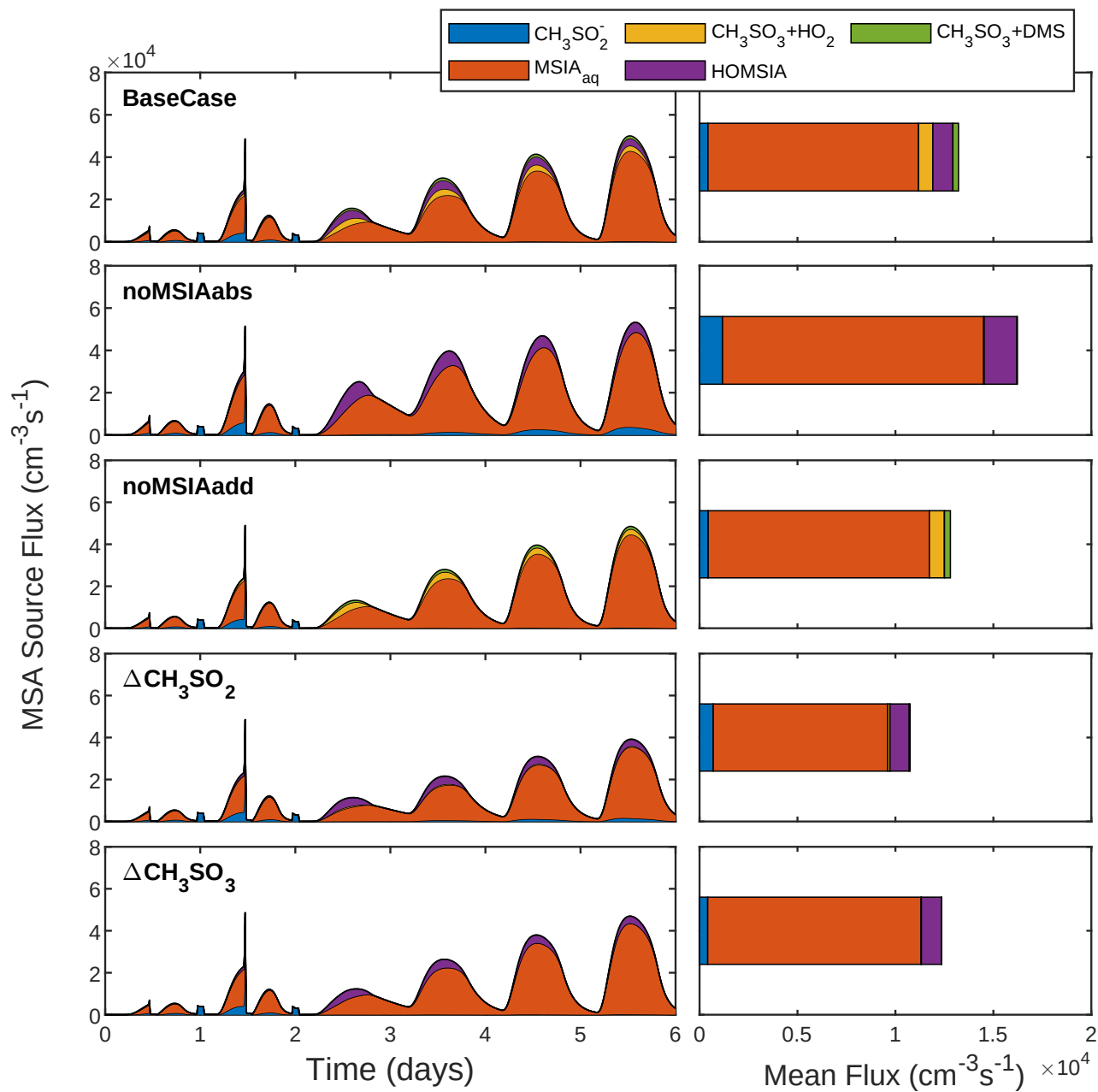


Figure S88. MSA source flux from CH₃SO₂⁻ and MSIA_{aq} in the aqueous-phase in addition to CH₃SO₃ via HO₂, CH₃SO₃ via DMS and HOMSA in the gas-phase for the BaseCase simulation and the noMSIAabs, noMSIAadd, ΔCH₃SO₂ and ΔCH₃SO₃ sensitivity runs.

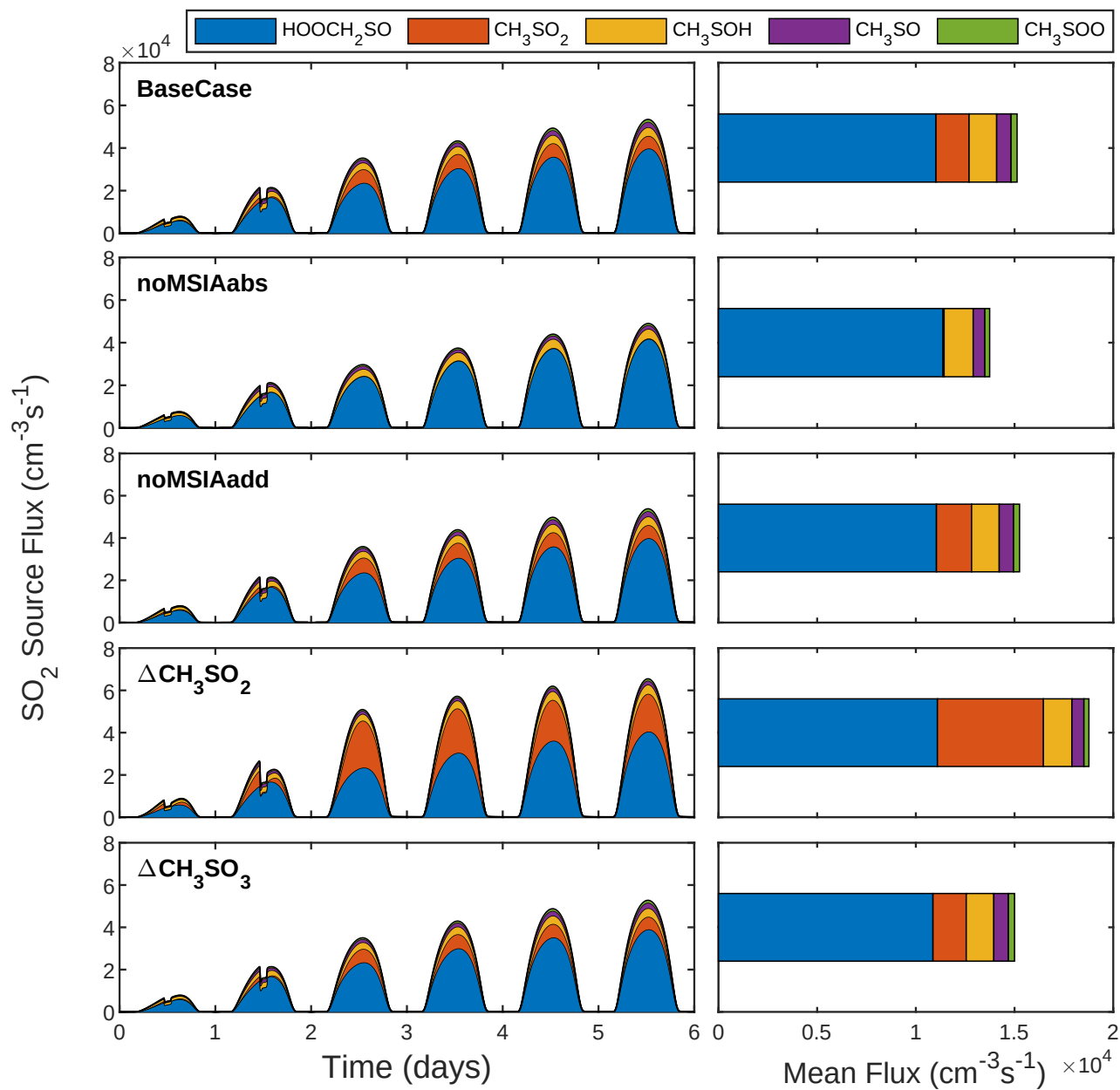


Figure S89. SO₂ source flux from HOOCH₂SO, CH₃SO₂, CH₃SOH, CH₃SO and CH₃SOO for the BaseCase simulation and the noMSIAabs, noMSIAadd, $\Delta\text{CH}_3\text{SO}_2$ and $\Delta\text{CH}_3\text{SO}_3$ sensitivity runs. Reactions that contribute < 1% of the total source flux are not displayed in the figure.

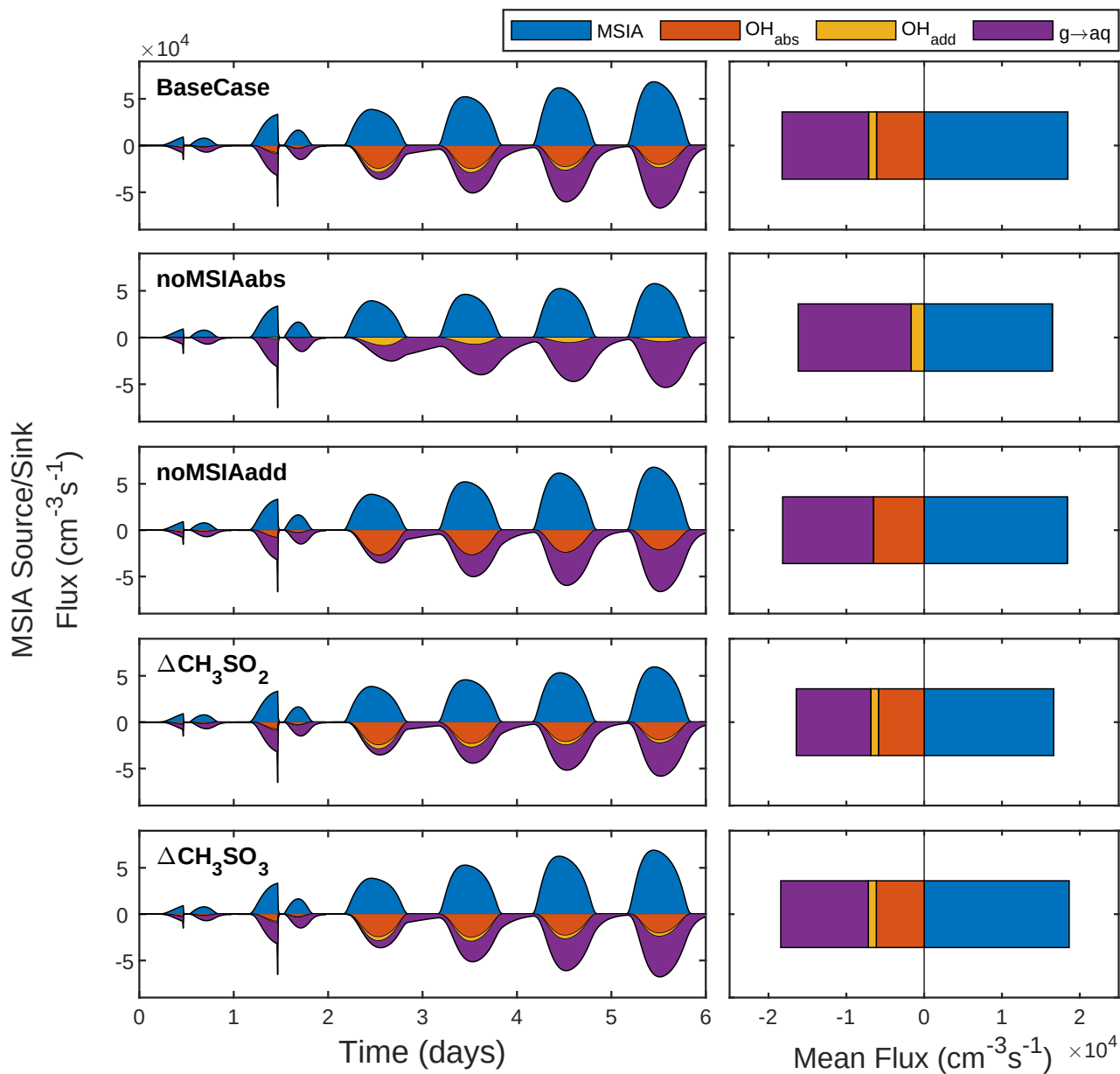


Figure S90. MSIA source/sink flux from DMSO and via reaction with OH (abstraction), OH (addition) and gas-aqueous phase uptake for the BaseCase simulation and the noMSIAabs, noMSIAadd, $\Delta\text{CH}_3\text{SO}_2$ and $\Delta\text{CH}_3\text{SO}_3$ sensitivity runs. Reactions that contribute < 1% of the total source/sink flux are not displayed in the figure.

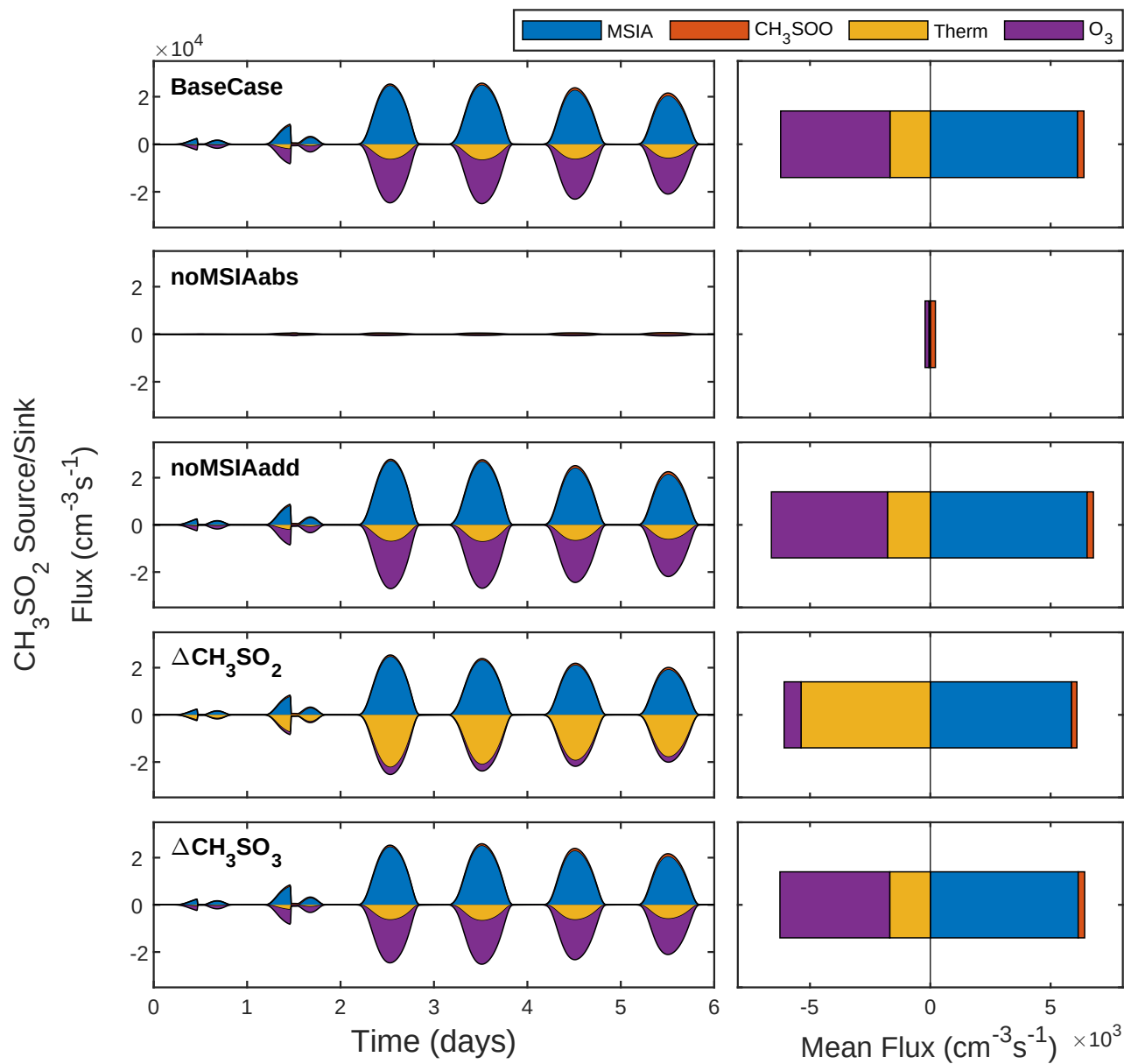


Figure S91. CH_3SO_2 source/sink flux from MSIA, CH_3SOO and via thermal decomposition and reaction with O_3 for the BaseCase simulation and the noMSIAabs, noMSIAadd, $\Delta\text{CH}_3\text{SO}_2$ and $\Delta\text{CH}_3\text{SO}_3$ sensitivity runs. Reactions that contribute $< 1\%$ of the total source/sink flux are not displayed in the figure.

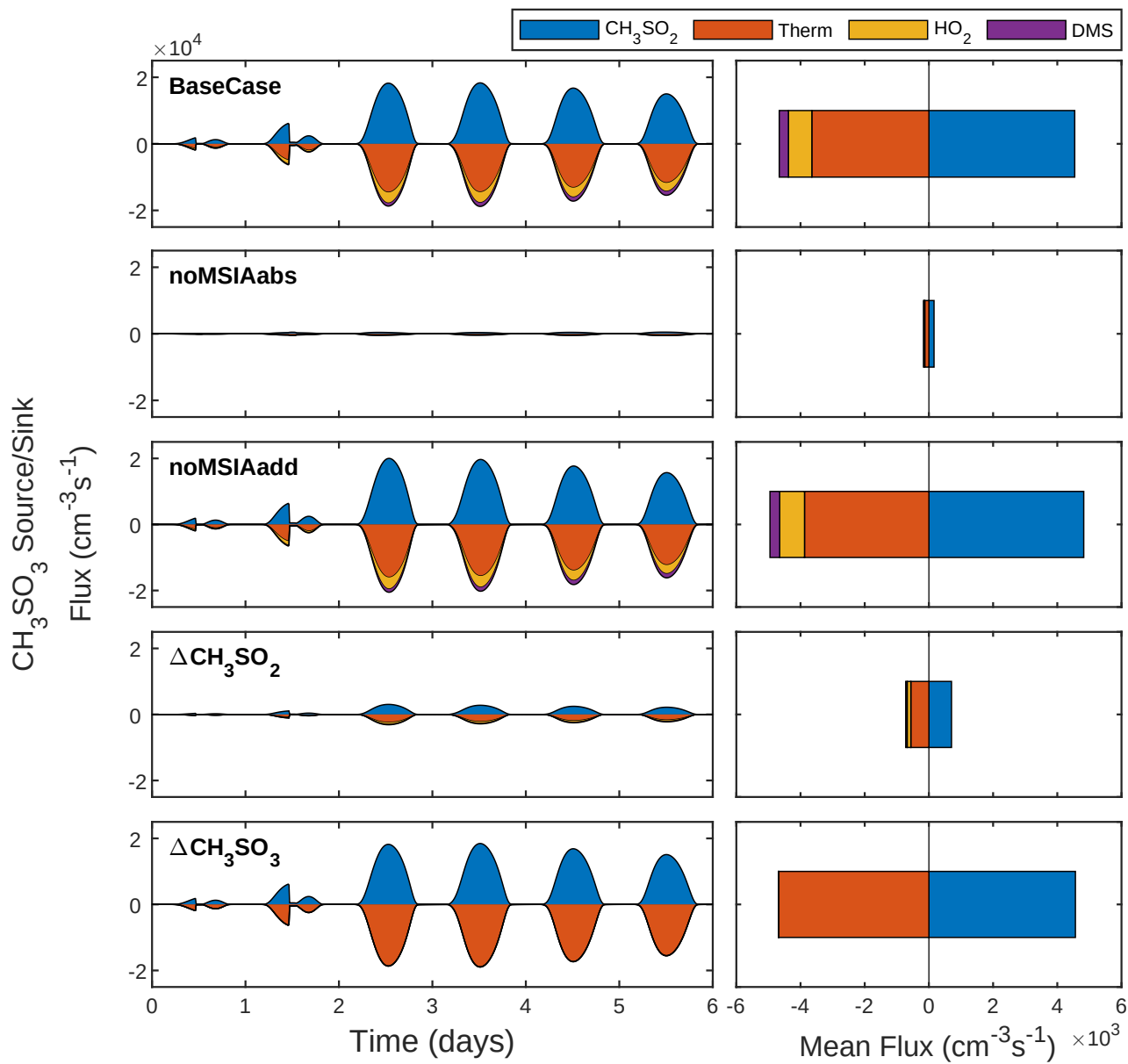


Figure S92. CH_3SO_3 source/sink flux from CH_3SO_2 , via thermal decomposition and reaction with HO_2 and DMS for the BaseCase simulation and the noMSIAabs, noMSIAadd, $\Delta\text{CH}_3\text{SO}_2$ and $\Delta\text{CH}_3\text{SO}_3$ sensitivity runs. Reactions that contribute $< 1\%$ of the total source/sink flux are not displayed in the figure.

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