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Supplement of

CAPRAM reduction towards an operational multiphase halogen and dimethyl sulfide chemistry treatment in the chemistry transport model COSMO-MUSCAT(5.04e)

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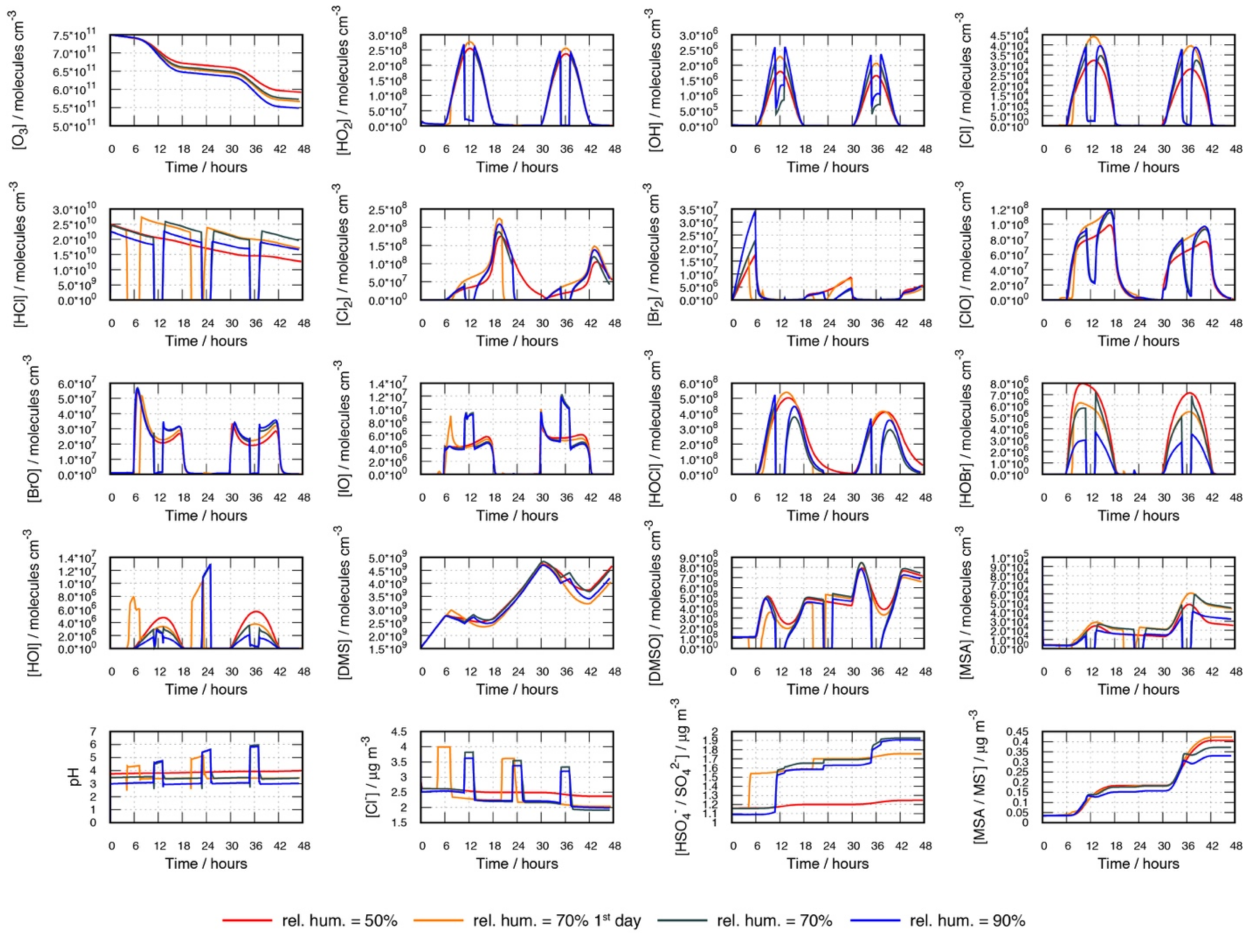

Figure S1 **Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the summer simulations at 15° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.**

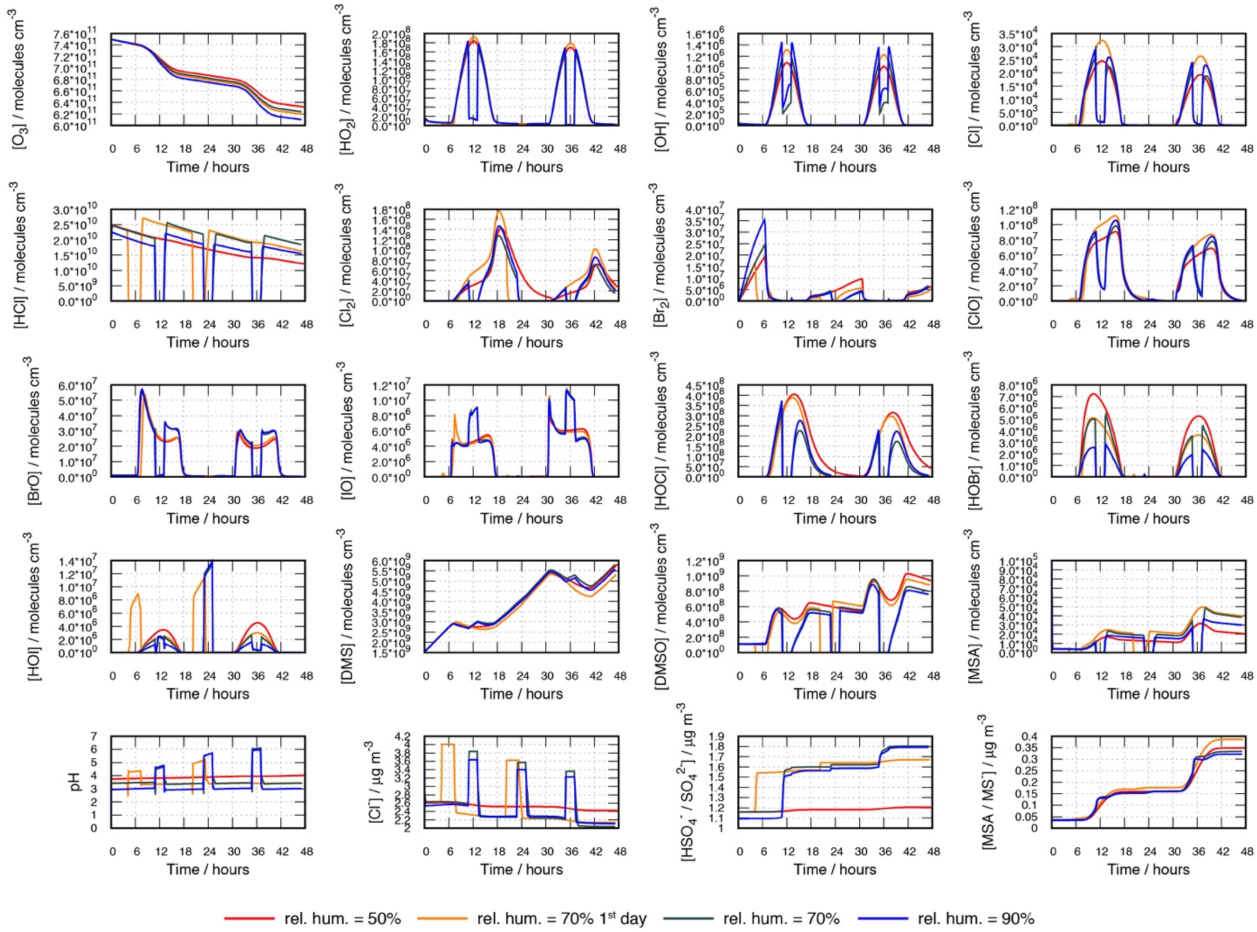

Figure S2 **Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the winter simulations at 15° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.**

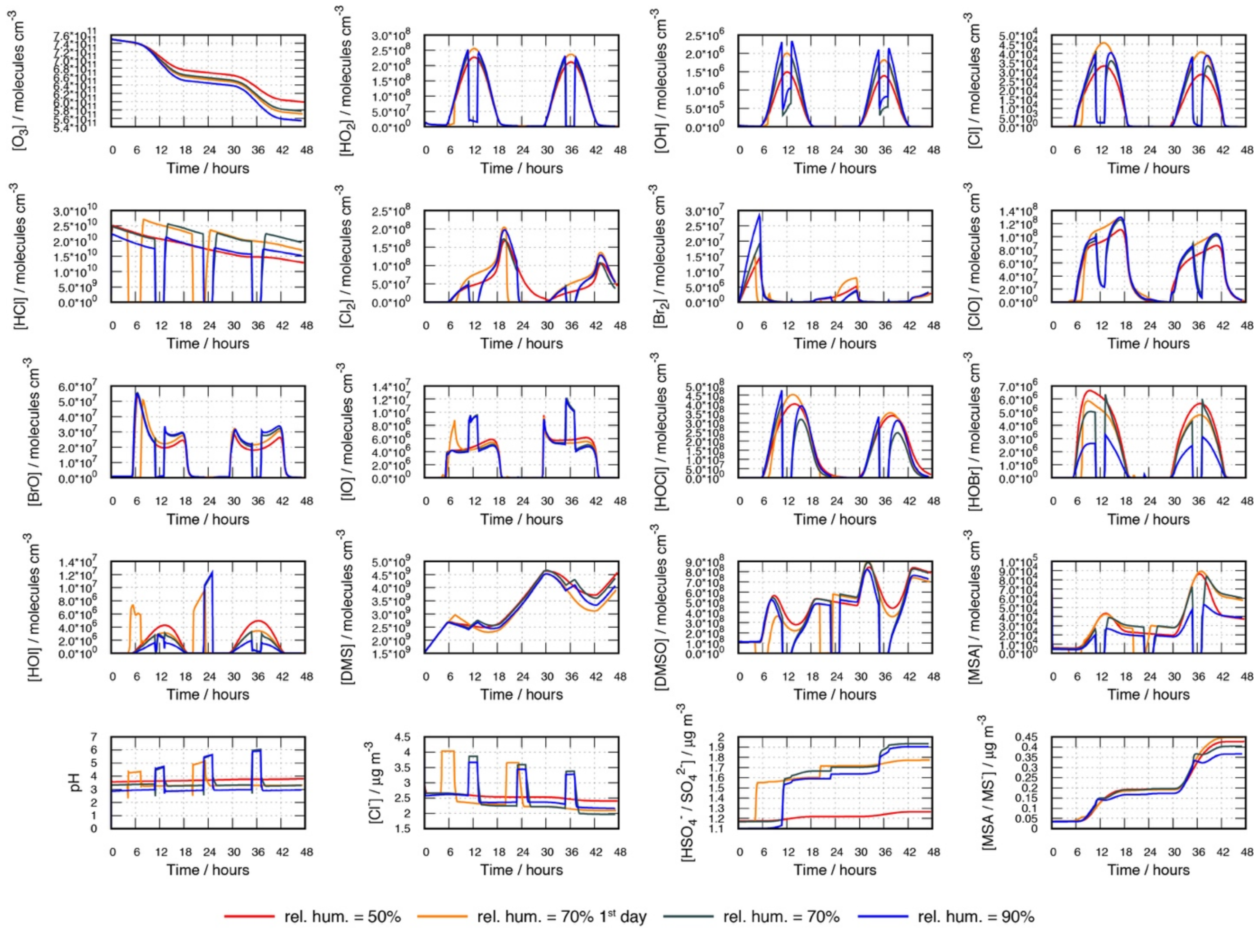

Figure S3 **Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the summer simulations at 30° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.**

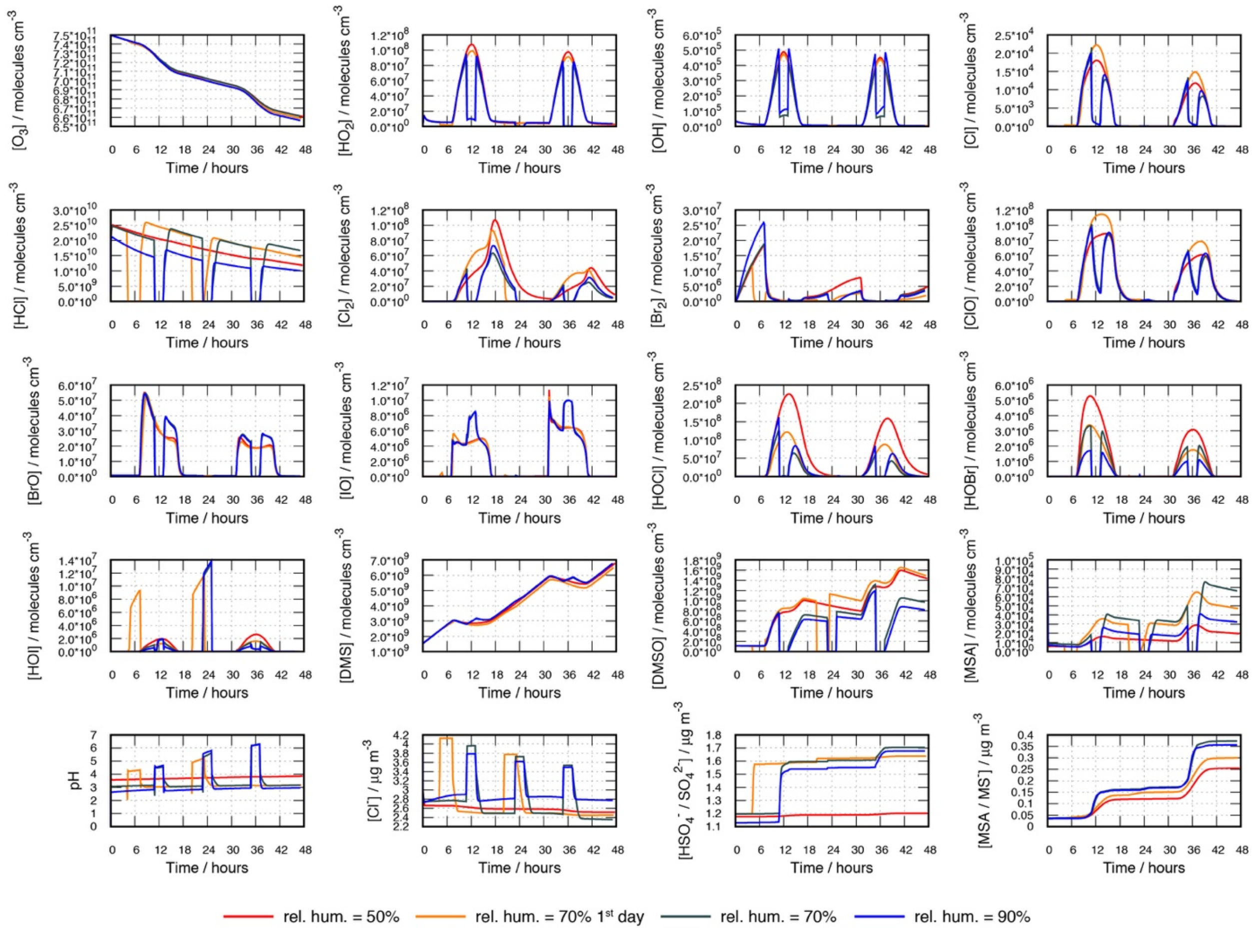

Figure S4 **Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the winter simulations at 30° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.**

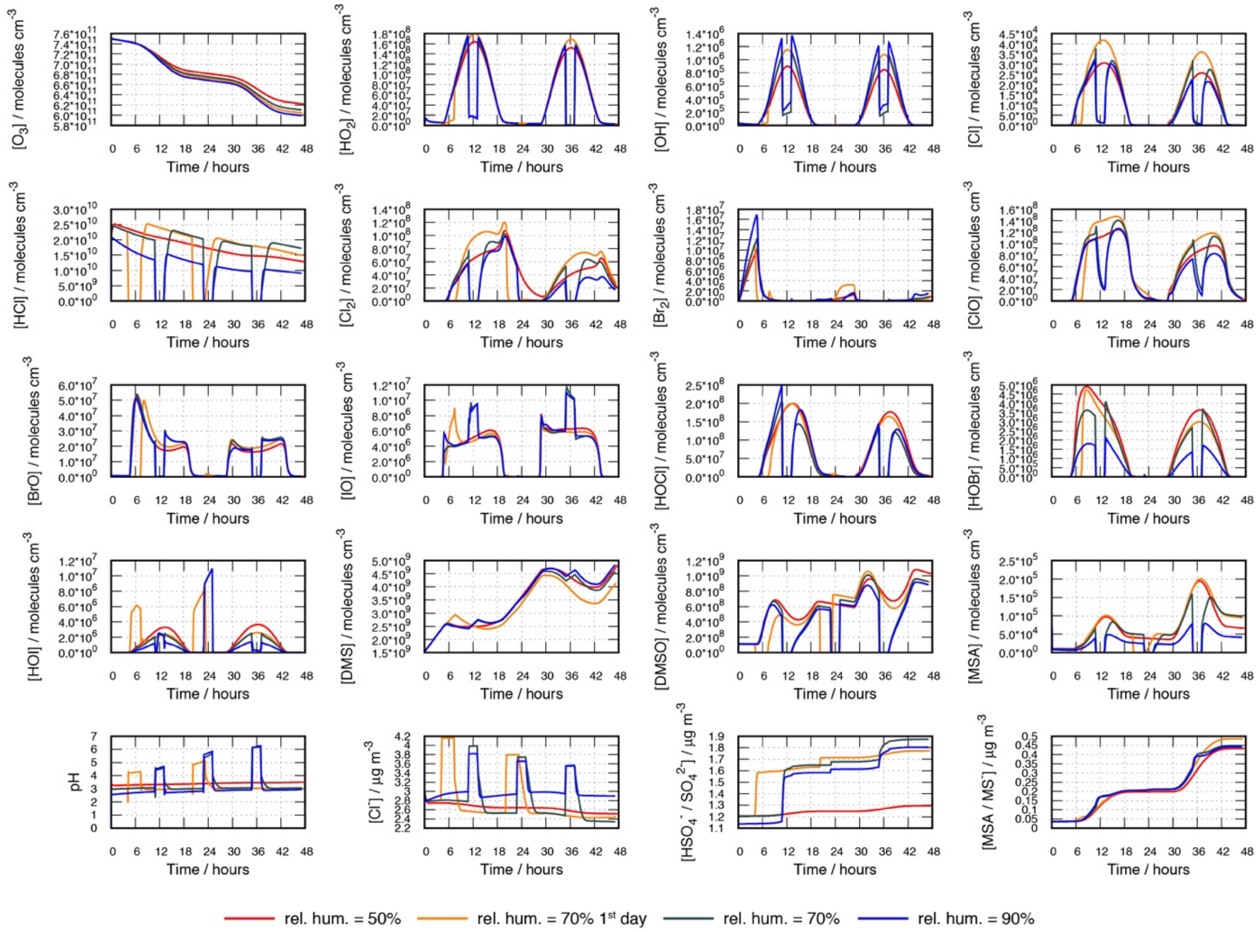

Figure S5 Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the summer simulations at 45° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.

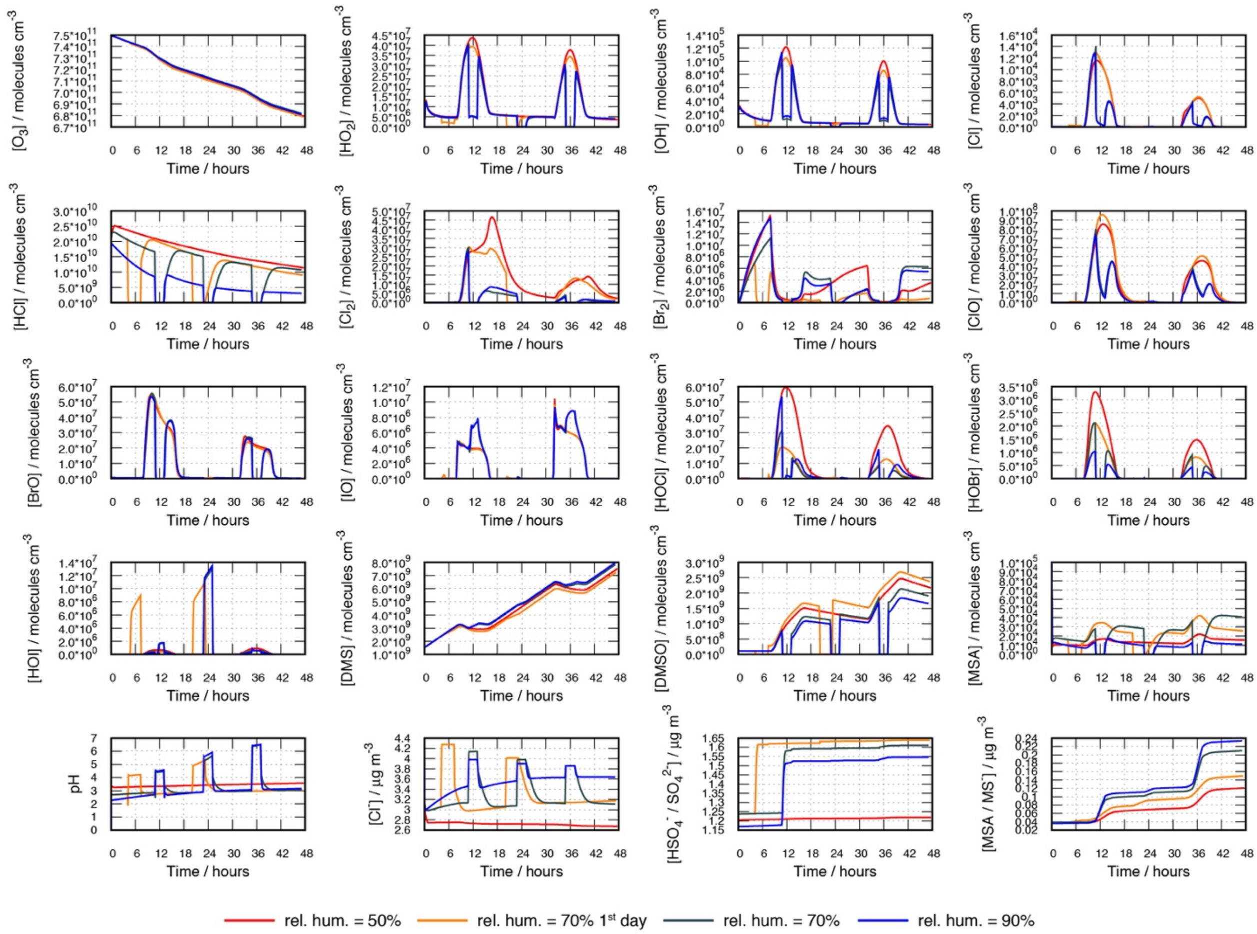

Figure S6 Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the winter simulations at 45° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.

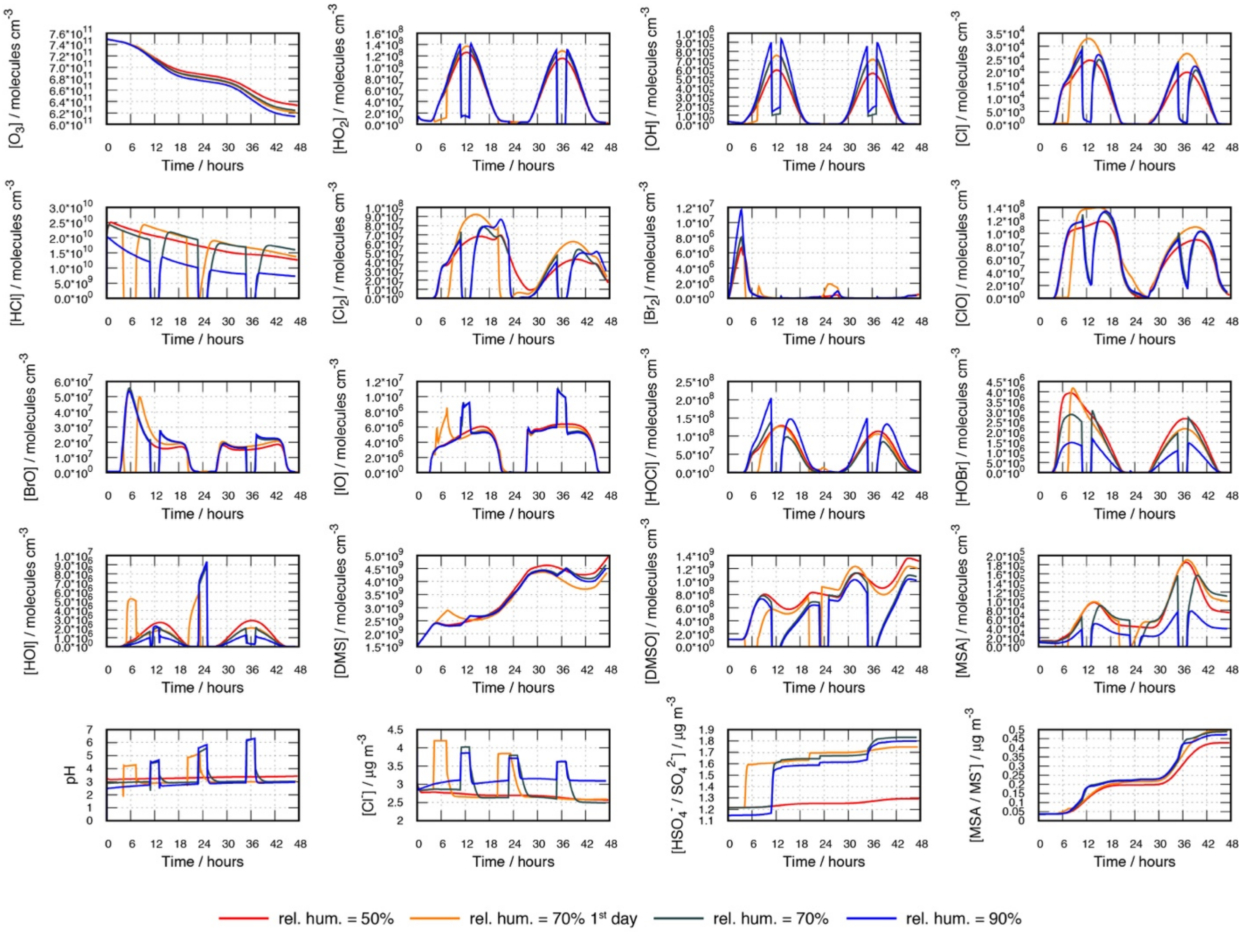

Figure S7 **Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the summer simulations at 60° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.**

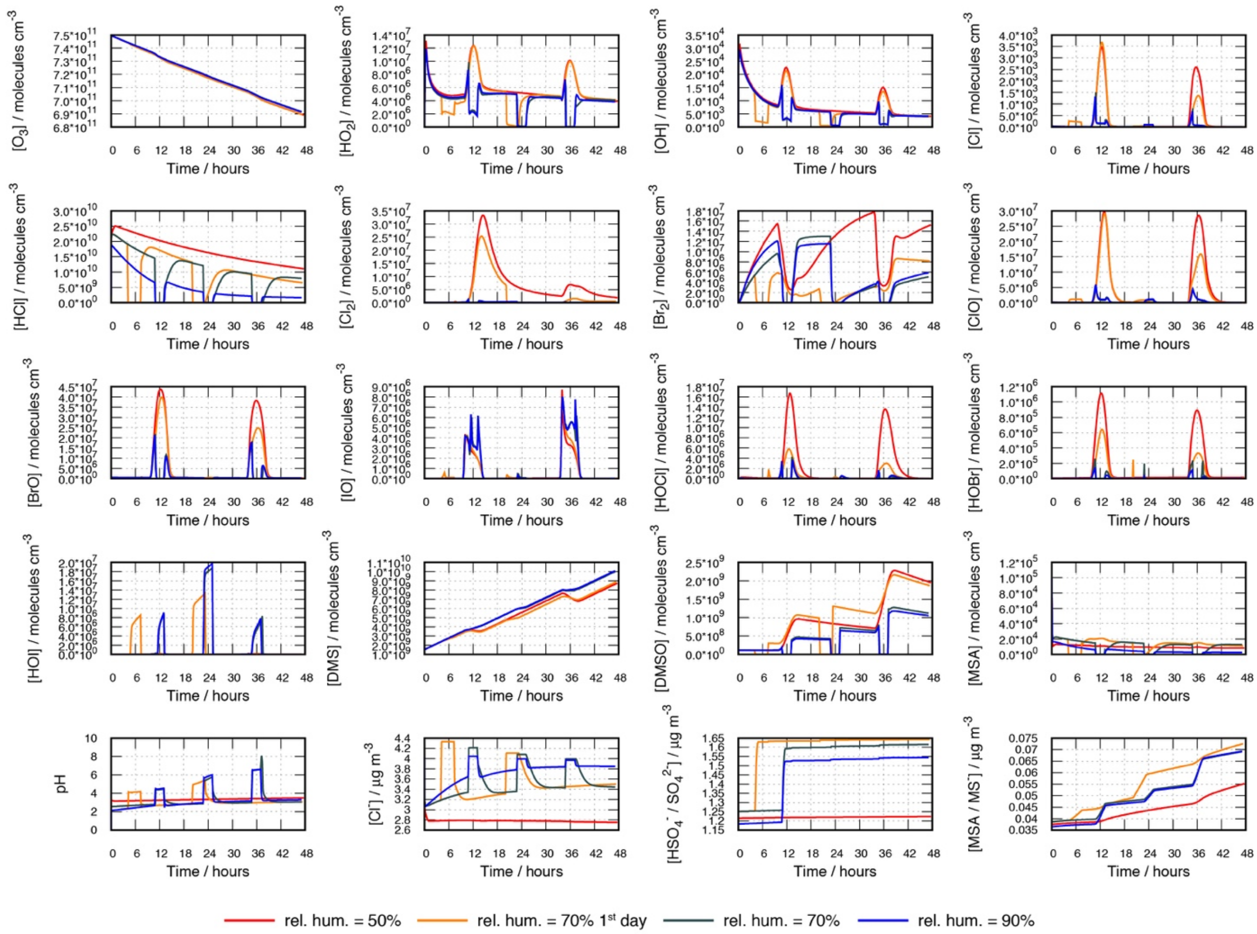

Figure S8 **Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the winter simulations at 60° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.**

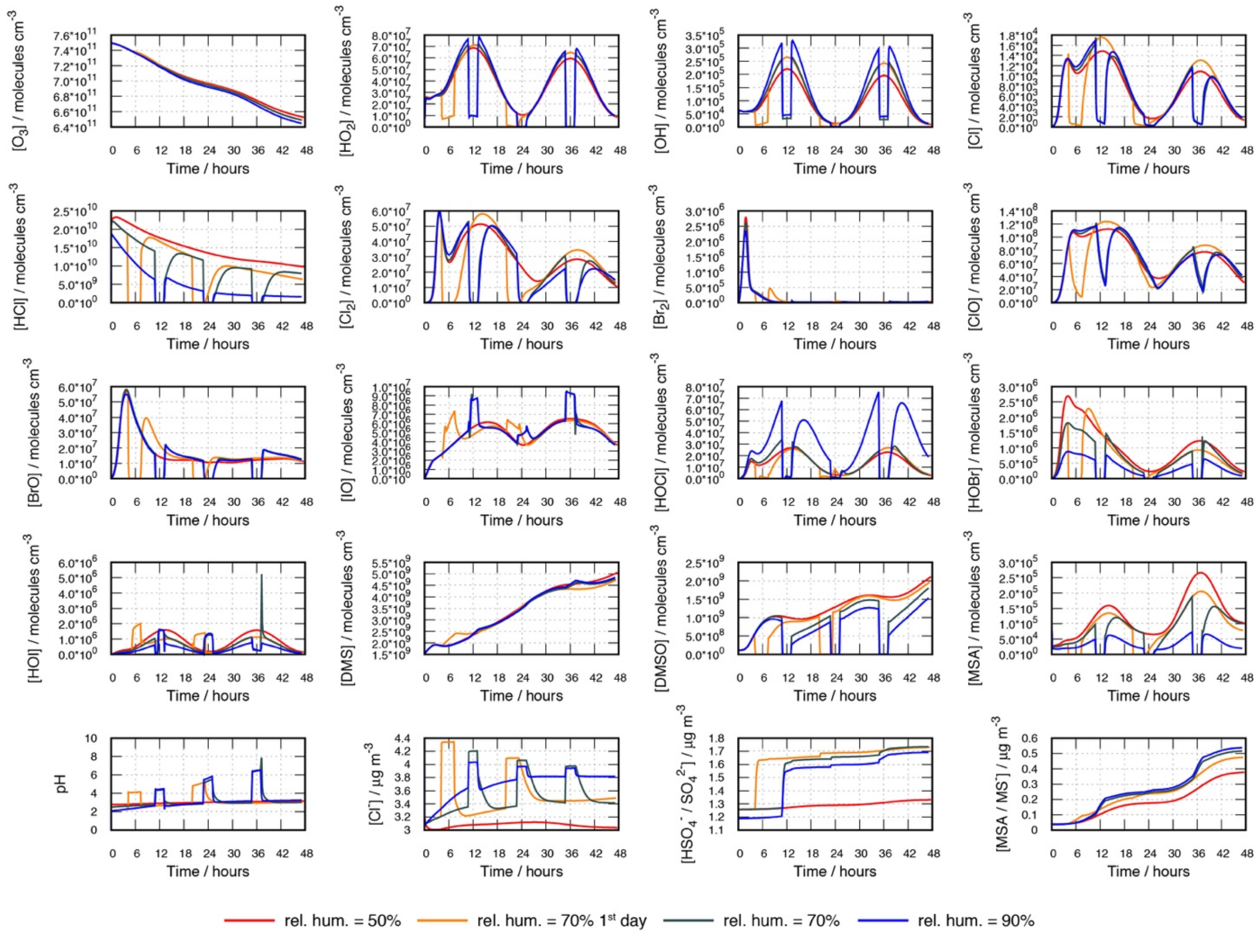

Figure S9 **Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the summer simulations at 75° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.**

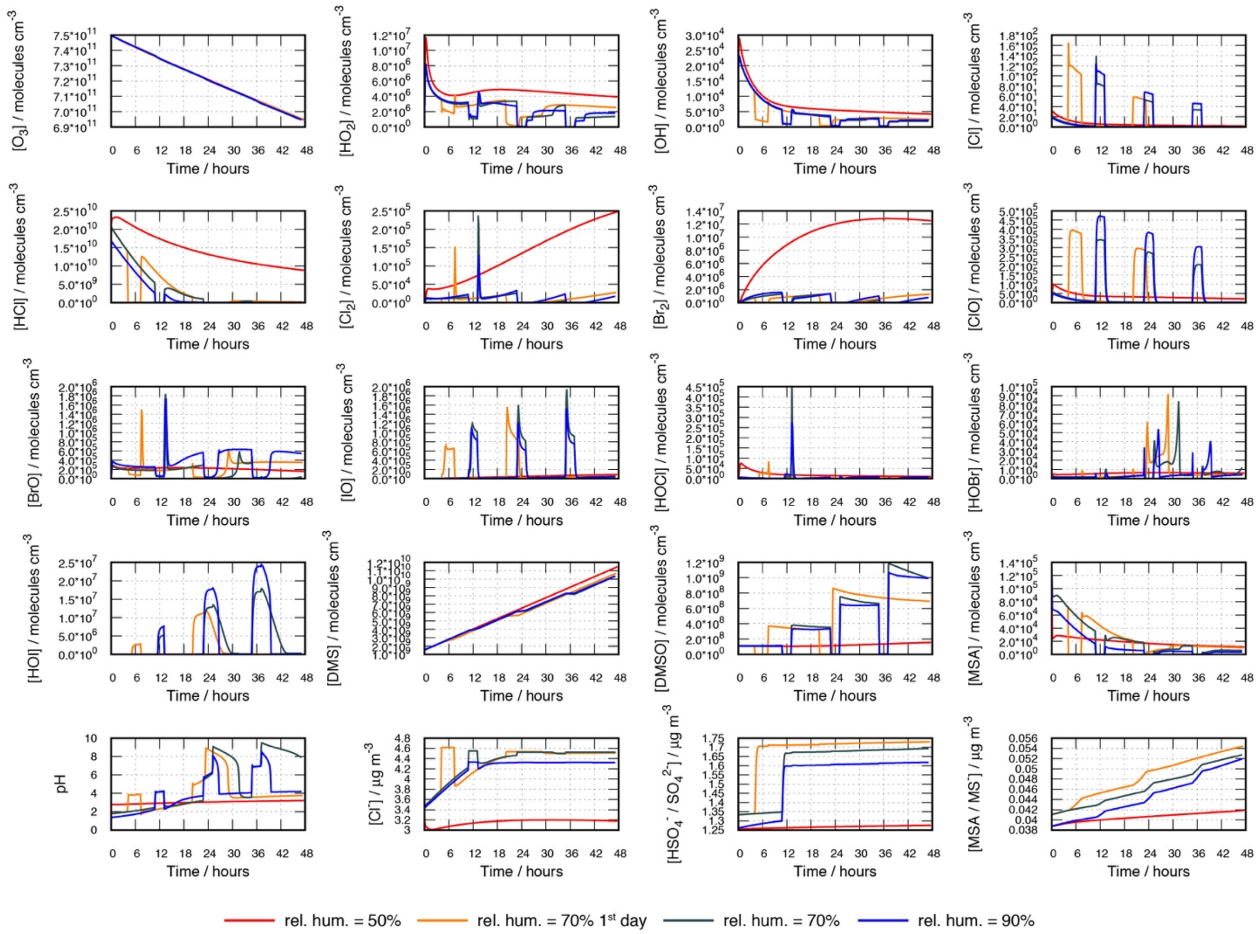

Figure S10 **Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the winter simulations at 75° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.**

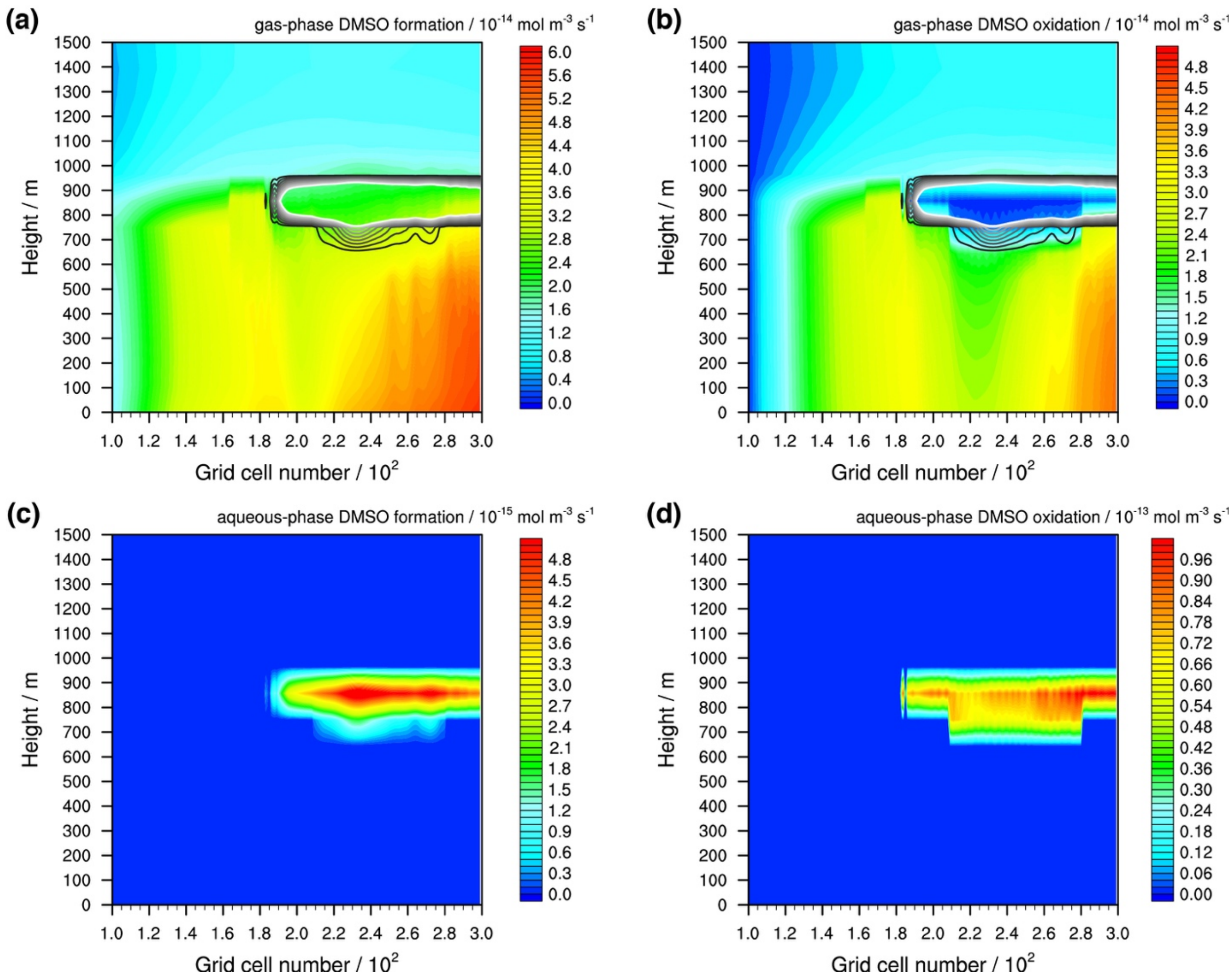

Figure S11 Modelled formation rate of DMSO in (a) the gas phase and (c) the aqueous phase together with the modelled oxidation rate in (b) the gas phase and (d) the aqueous phase in the 'stable meteorological condition' simulation with stratiform clouds after 12 hours of modelling time. The x-axis represents the innermost horizontal grid cells divided by 100. The black contour lines represent the simulated clouds. The black line corresponds to a liquid water content of 0.01 g m^{-3} and the white line to 0.1 g m^{-3}. The area framed by the white line includes LWC above 0.1 g m^{-3}.

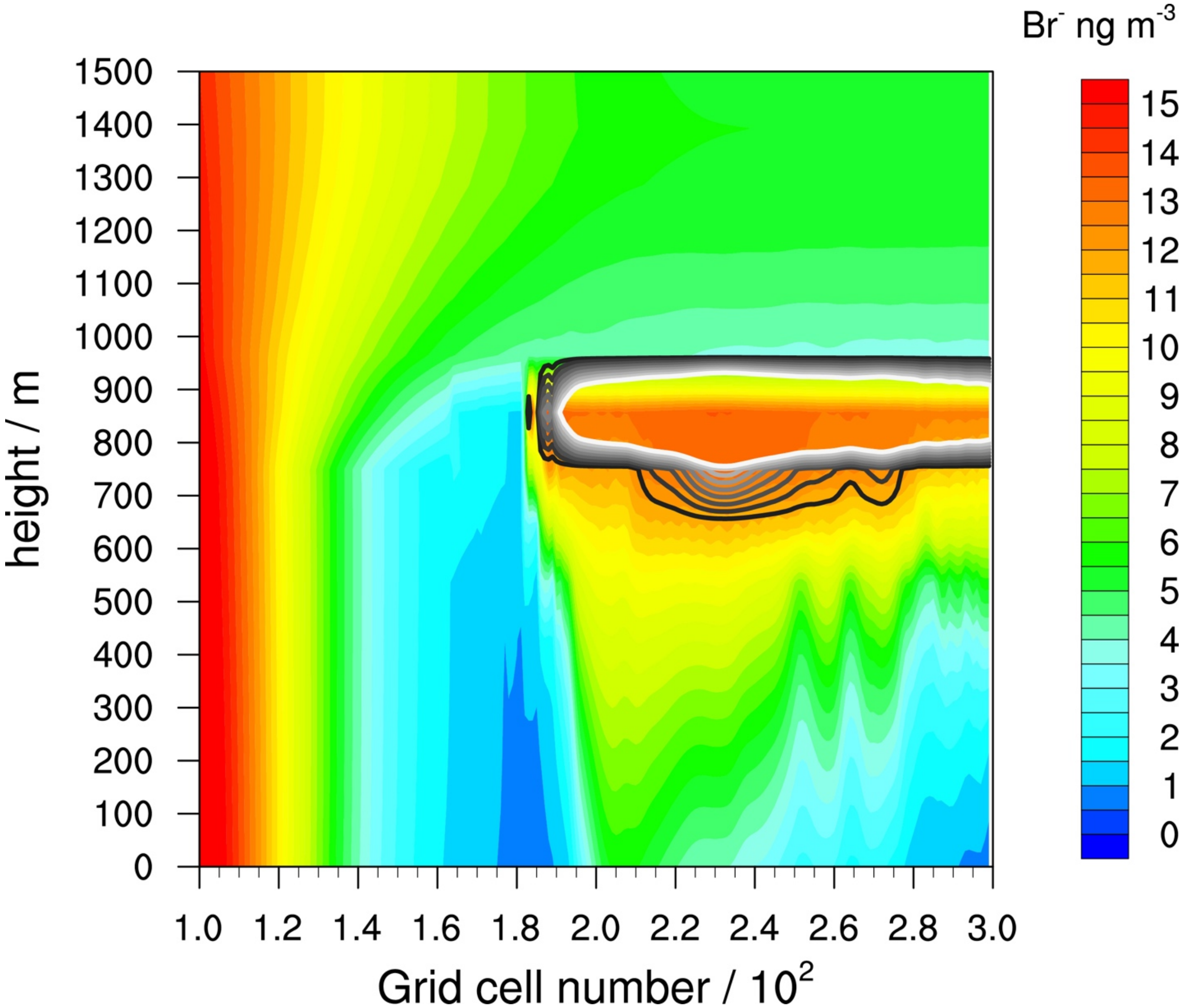

Figure S12 **Simulated aqueous-phase concentration of bromide in the 'stable meteorological condition' simulation with stratiform clouds after 12 hours of modelling time. The x-axis represents the innermost horizontal grid cells divided by 100. The black contour lines represent the simulated clouds. The black line corresponds to a liquid water content of 0.01 g m^{-3} and the white line to 0.1 g m^{-3}. The area framed by the white line includes LWC above 0.1 g m^{-3}. The initial background concentration is at about 16 ng m^{-3}.**

Table S1 **Implemented dry deposition, initial concentrations, and emission rates of chemical species for the open ocean simulation with COSMO-MUSCAT. Details on the dry deposition velocities are given in the previous CAPRAM studies Bräuer et al. (2013), Hoffmann et al. (2016) and Hoffmann et al. (2019a). Details on the initial concentrations and emission rates are given in Bräuer et al. (2013) and Hoffmann et al. (2016). In the term of I_2 and HOI, emission rates are derived from Prados-Roman et al. (2015). Aerosol initial concentrations are calculated from the SPACCIM simulations and were provided in the previous CAPRAM study Bräuer et al. (2013).**

Specie	Dry deposition / s^{-1}	Initial concentration / molecules cm^{-3}	Emission rates / mol m^{-2} s^{-1}	Aerosol initial concentration / mol m^{-3}
NH_3	$1.0 \cdot 10^{-2}$	$1.28 \cdot 10^{9}$	$7.589 \cdot 10^{-10}$	
NO	$2.0 \cdot 10^{-4}$	$2.50 \cdot 10^{8}$	$4.151 \cdot 10^{-12}$	
NO_2	$2.0 \cdot 10^{-4}$	$5.00 \cdot 10^{8}$		
NO_3	$1.0 \cdot 10^{-2}$			
N_2O_5	$1.0 \cdot 10^{-2}$			
HONO		$2.50 \cdot 10^{8}$		
HNO_3	$7.0 \cdot 10^{-3}$	$2.00 \cdot 10^{9}$		
HO_2NO_2	$5.0 \cdot 10^{-3}$			
O_3	$1.5 \cdot 10^{-3}$	$7.50 \cdot 10^{11}$		
CO	$1.0 \cdot 10^{-3}$	$4.25 \cdot 10^{12}$	$1.416 \cdot 10^{-9}$	
CO_2		$1.02 \cdot 10^{16}$		
SO_2	$8.7 \cdot 10^{-3}$	$2.55 \cdot 10^{9}$		
SULF	$1.0 \cdot 10^{-2}$			
H_2		$1.28 \cdot 10^{13}$		
H_2O_2	$5.0 \cdot 10^{-3}$	$1.50 \cdot 10^{10}$		
CH_4		$4.50 \cdot 10^{13}$	$2.923 \cdot 10^{-11}$	
C_2H_6		$1.28 \cdot 10^{10}$	$1.661 \cdot 10^{-13}$	
C_3H_8		$2.31 \cdot 10^{10}$	$3.321 \cdot 10^{-13}$	
C_2H_2		$2.42 \cdot 10^{9}$	$1.661 \cdot 10^{-13}$	
C_2H_4		$2.55 \cdot 10^{9}$	$3.985 \cdot 10^{-12}$	
C_3H_6			$1.661 \cdot 10^{-12}$	
BIGENE		$9.50 \cdot 10^{8}$		
HCHO	$5.0 \cdot 10^{-3}$	$5.00 \cdot 10^{9}$	$2.956 \cdot 10^{-14}$	
CH_3CHO		$1.40 \cdot 10^{8}$	$1.513 \cdot 10^{-10}$	
C_2H_5CHO		$5.13 \cdot 10^{9}$	$9.083 \cdot 10^{-11}$	
HYAC		$3.83 \cdot 10^{8}$	$4.151 \cdot 10^{-12}$	

Specie	Dry deposition / s^{-1}	Initial concentration / molecules cm^{-3}	Emission rates / mol m^{-2} s^{-1}	Aerosol initial concentration / mol m^{-3}
CH_3COCH_3		$1.10 \cdot 10^{10}$	$6.320 \cdot 10^{-12}$	
MEK		$6.89 \cdot 10^{8}$	$7.124 \cdot 10^{-16}$	
GLYOXAL		$2.55 \cdot 10^{8}$		
CH_3COCHO		$2.55 \cdot 10^{8}$		
CH_3OOH	$2.5 \cdot 10^{-3}$	$5.00 \cdot 10^{9}$		
CH_3CH_2OOH		$2.55 \cdot 10^{9}$		
CH_3COOOH		$2.55 \cdot 10^{7}$		
PAN	$1.0 \cdot 10^{-4}$	$2.50 \cdot 10^{8}$		
CH_3OH	$1.0 \cdot 10^{-2}$	$1.40 \cdot 10^{10}$	$9.797 \cdot 10^{-16}$	
CH_3CH_2OH	$5.0 \cdot 10^{-3}$	$2.00 \cdot 10^{9}$	$1.015 \cdot 10^{-11}$	
HCOOH	$1.0 \cdot 10^{-2}$	$6.25 \cdot 10^{9}$		
CH_3COOH		$5.00 \cdot 10^{9}$	$1.278 \cdot 10^{-12}$	
C_5H_8		$1.28 \cdot 10^{9}$	$2.341 \cdot 10^{-12}$	
APIN		$4.53 \cdot 10^{8}$	$2.541 \cdot 10^{-14}$	
BPIN		$3.02 \cdot 10^{8}$		
$CHBr_3$		$3.83 \cdot 10^{7}$	$2.225 \cdot 10^{-13}$	
C_3H_7I		$1.63 \cdot 10^{7}$	$8.170 \cdot 10^{-15}$	
CH_2I_2		$2.55 \cdot 10^{5}$	$1.876 \cdot 10^{-13}$	
CH_3I		$2.04 \cdot 10^{7}$	$2.458 \cdot 10^{-13}$	
CH_2ClI		$2.55 \cdot 10^{5}$	$1.524 \cdot 10^{-13}$	
CH_2BrI		$8.93 \cdot 10^{5}$	$8.751 \cdot 10^{-14}$	
HCl	$2.0 \cdot 10^{-2}$	$2.50 \cdot 10^{9}$		
HOCl	$2.0 \cdot 10^{-3}$			
$ClNO_2$	$1.0 \cdot 10^{-2}$			
$ClNO_3$	$1.0 \cdot 10^{-2}$			
HBr	$2.0 \cdot 10^{-2}$			
HOBr	$1.6 \cdot 10^{-3}$			
$BrNO_2$	$1.0 \cdot 10^{-2}$			
$BrNO_3$	$5.0 \cdot 10^{-3}$			
I_2			$1.744 \cdot 10^{-14}$	
HOI	$1.0 \cdot 10^{-2}$		$3.321 \cdot 10^{-13}$	

Specie	Dry deposition / s^{-1}	Initial concentration / molecules cm^{-3}	Emission rates / mol m^{-2} s^{-1}	Aerosol initial concentration / mol m^{-3}
INO_3	$1.0\cdot10^{-2}$			
I_2O_2	$1.0\cdot10^{-2}$			
I_2O_3	$1.0\cdot10^{-2}$			
I_2O_4	$1.0\cdot10^{-2}$			
DMS		$1.53\cdot10^{9}$	$1.026\cdot10^{-10}$	
DMSO	$5.0\cdot10^{-3}$			
$DMSO_2$	$5.0\cdot10^{-3}$			
MSA	$5.0\cdot10^{-3}$			
SO_4^{2-}				$1.05\cdot10^{-8}$
NO_3^-				$2.05\cdot10^{-9}$
Cl^-				$9.76\cdot10^{-8}$
Br^-				$2.14\cdot10^{-10}$
NH_4^+				$5.72\cdot10^{-9}$
Mn^{3+}				$3.93\cdot10^{-15}$
Fe^{3+}				$4.80\cdot10^{-15}$
Cu^{2+}				$1.72\cdot10^{-13}$
$HC_2O_4^-$				$3.94\cdot10^{-11}$
MSA				$3.26\cdot10^{-10}$
H^+				$1.00\cdot10^{-11}$

Table S2 Implemented gas-phase reactions in the CAPRAM-DM1.0red.

Nr.	Reaction	Rate constant[(a)]	Reference
D1	$DMS + OH \rightarrow CH_3SCH_2O_2 - O_2$	$k = 1.12 \cdot 10^{-11} \exp(-250/T)$	IUPAC, Atkinson et al. (2004)
D2	$DMS + OH \rightarrow 0.9\ DMSO + 0.9\ HO_2 + 0.1\ CH_3SOH + 0.1\ CH_3O_2 - O_2$	**(1)**	see description at the table end
D3	$DMS + NO_3 \rightarrow CH_3SCH_2O_2 - O_2$	$k = 1.90 \cdot 10^{-13} \exp(520/T)$	IUPAC, Atkinson et al. (2004)
D4	$DMS + Cl \rightarrow 0.82\ CH_3SCH_2O_2 + 0.82\ HCl + 0.18\ DMSO + 0.18\ ClO - O_2$	$k = 1.88 \cdot 10^{-10}$	IUPAC, Urbanski and Wine (1999)
D5	$DMS + ClO \rightarrow 0.73\ Cl + 0.73\ DMSO + 0.27\ HOCl + 0.27\ CH_3SCH_2O_2 - 0.27\ O_2$	$k = 1.70 \cdot 10^{-15} \exp(340/T)$	IUPAC
D6	$DMS + BrO \rightarrow DMSO + Br$	$k = 1.50 \cdot 10^{-14} \exp(1000/T)$	IUPAC
D7	$DMS + Cl_2 \rightarrow CH_3SCH_2Cl + HCl$	$k = 3.40 \cdot 10^{-14}$	Dyke et al. (2005)
D8	$DMS + IO \rightarrow DMSO + I$	$k = 3.30 \cdot 10^{-13} \exp(-925/T)$	IUPAC
D9	$CH_3SCH_2O_2 + HO_2 \rightarrow CH_3SCH_2OOH + O_2$	$k = 1.13 \cdot 10^{-13} \exp(1300/T)$	MCMv3.2, Rickard et al. (21.10.2013)
D10	$CH_3SCH_2O_2 + NO \rightarrow CH_3S + HCHO + NO_2$	$k = 4.90 \cdot 10^{-12} \exp(260/T)$	MCMv3.2, Rickard et al. (21.10.2013)
D11	$CH_3SCH_2O_2 + NO_3 \rightarrow CH_3S + HCHO + NO_2 + O_2$	$k = 2.30 \cdot 10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)
D12	$CH_3SCH_2O_2 + CH_3O_2 \rightarrow 0.89\ CH_3S + 0.89\ HCHO + 0.11\ CH_3SCHO + O_2$	$k = 5.00 \cdot 10^{-13} \exp(400/T)$	In accordance to MCMv3.2 RO2 reaction
D13	$CH_3SCH_2Cl + OH \rightarrow CH_3SOH + ClCH_2O_2 - O_2$	$k = 2.50 \cdot 10^{-12}$	Shallcross et al. (2006)
D14	$CH_3SCH_2OOH + OH \rightarrow CH_3SCHO + OH + H_2O$	$k = 7.03 \cdot 10^{-11}$	MCMv3.2, Rickard et al. (21.10.2013)
D15	$CH_3SCHO + OH \rightarrow CH_3S + CO + H_2O$	$k = 1.11 \cdot 10^{-11}$	MCMv3.2, Rickard et al. (21.10.2013)
D16	$DMSO + OH \rightarrow MSIA + CH_3O_2 - O_2$	$k = 6.10 \cdot 10^{-12} \exp(800/T)$	MCMv3.2, Rickard et al. (21.10.2013)
D17	$DMSO + NO_3 \rightarrow DMSO_2 + NO_2$	$k = 2.90 \cdot 10^{-13}$	Sander et al. (2006)
D18	$DMSO + Cl \rightarrow 0.43\ DMSO_2 + 0.43\ ClO + 0.57\ CH_3SO + 0.57\ HCHO + 0.57\ HCl - 0.43\ O_2$	$k = 1.45 \cdot 10^{-11}$	Falbe-Hansen et al. (2000); Nicovich et al. (2006); Kleissas et al. (2007)
D19	$DMSO + BrO \rightarrow CH_3SO_2CH_3 + Br$	$k = 1.00 \cdot 10^{-14}$	Ballesteros et al. (2002)
D20	$CH_3SOH + OH \rightarrow CH_3SO + H_2O$	$k = 5.00 \cdot 10^{-11}$	Lucas and Prinn (2002a)
D21	$CH_3S + O_3 \rightarrow CH_3SO + O_2$	$k = 1.15 \cdot 10^{-12} \exp(430/T)$	MCMv3.2, Rickard et al. (21.10.2013)
D22	$CH_3S + O_2 \rightarrow CH_3O_2 + SO_2 - O_2$	**(2)**	see description at the table end
D23	$CH_3S + O_2 \rightarrow CH_3SO_2$	**(3)**	see description at the table end
D24	$MSIA + OH \rightarrow CH_3O_2 + SO_2 + H_2O - O_2$	$k = 9.00 \cdot 10^{-11}$	MCMv3.2, Rickard et al. (21.10.2013)
D25	$CH_3SO + O_3 \rightarrow CH_3O_2 + SO_2$	$k = 4.00 \cdot 10^{-13}$	MCMv3.2, Rickard et al. (21.10.2013)
D26	$CH_3SO_2 + O_3 \rightarrow CH_3SO_3 + O_2$	$k = 3.00 \cdot 10^{-13}$	MCMv3.2, Rickard et al. (21.10.2013)

Nr.	Reaction	Rate constant[(a)]	Reference
D27	$CH_3SO_2 \rightarrow CH_3O_2 + SO_2 - O_2$	$k = 5.00 \cdot 10^{+13} \exp(-9673/T)$	MCMv3.2, Rickard et al. (21.10.2013)
D28	$CH_3SO_3 + HO_2 \rightarrow MSA + O_2$	$k = 5.00 \cdot 10^{-11}$	MCMv3.2, Rickard et al. (21.10.2013)
D29	$CH_3SO_3 \rightarrow CH_3O_2 + SULF - H_2O - O_2$	$k = 5.00 \cdot 10^{+13} \exp(-9946/T)$	MCMv3.2, Rickard et al. (21.10.2013)
Photolysis reactions			
D30	$CH_3SCH_2OOH \rightarrow CH_3S + HCHO + OH$	$J = 7.649 \cdot 10^{-06} \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	MCMv3.2, Rickard et al. (21.10.2013)
D31	$CH_3SCHO \rightarrow CH_3S + CO + HO_2 - O_2$	$J = 2.792 \cdot 10^{-05} \cos(\chi)^{0.805} \exp(-0.338/\cos(\chi))$	MCMv3.2, Rickard et al. (21.10.2013)
D32	$CH_3SCH_2Cl \rightarrow CH_3S + ClCH_2O_2 - O_2$	$J = 1.458 \cdot 10^{-04} \cos(\chi)^{0.314} \exp(-0.641/\cos(\chi))$	Hoffmann et al. (2016)

(a) k^{2nd} in cm^3 $molecules^{-1}$ s^{-1}; k^{1st} in s^{-1}; J in s^{-1};

(1) $k = \frac{k1 \times k3}{k2 + k3}$ with $k1 = \frac{9.5 \times 10^{-39} \times [O_2] \times e^{5270/T}}{1 + 7.5 \times 10^{-29} \times [O_2] \times e^{5610/T}}$; $k2 = \frac{2.05 \times 10^{-14} \times [O_2] \times e^{2674/T}}{\left(1 + 5.5 \times 10^{-31} \times [O_2] \times e^{7460/T}\right) \times T}$; rate calculated after Atkinson et al. (2004); Lucas and Prinn (2002b); Sander et al. (2006)

(2) $k = \frac{k1}{1 + k2}$ with $k1 = 1.92 \times 10^{-10} \times e^{-5730/T}$; $k2 = 1.60 \times 10^{6} \times e^{-7310/T}$; rate calculated after MCMv3.2, Rickard et al. (21.10.2013)

(3) $k = \frac{k1}{1 + k2}$ with $k1 = 3.43 \times 10^{-27} \times e^{-5140/T}$; $k2 = 2.86 \times 10^{-11} \times e^{-3560/T}$; rate calculated after Campolongo et al. (1999); Turnipseed et al. (1993); (Rickard et al., 21.10.2013)

Table S3 Implemented phase transfers in the CAPRAM-DM1.0red

② reactions that run in the cloud mode 'sub#1', ③ reactions that run in the aerosol mode 'sub#2'

Species	$K_{H\ (298\ K)}$[(a)]	$-\Delta H/R$[(b)]	Reference	α	Reference	$D_{g\ (298\ K)}$[(c)]	Reference
D33③ DMS	0.56	4480	Campolongo et al. (1999)	0.001	Zhu et al. (2006)	$1.08 \cdot 10^{-5}$	Fuller et al. (1966)
D34③ DMSO	$1.00 \cdot 10^{7}$	2580	Campolongo et al. (1999)	0.1	De Bruyn et al. (1994)	$1.01 \cdot 10^{-5}$	Fuller et al. (1966)
D35② $DMSO_2$	$1.00 \cdot 10^{7}$	5390	Campolongo et al. (1999)	0.1	De Bruyn et al. (1994)	$9.55 \cdot 10^{-6}$	Fuller et al. (1966)
D36② MSIA	$1.00 \cdot 10^{8}$	1760	between $DMSO_2$ and MSA	0.1	as for MSAa	$1.11 \cdot 10^{-5}$	Fuller et al. (1966)
D37② MSA	$5.09 \cdot 10^{13}$	1760	Campolongo et al. (1999)	0.1	De Bruyn et al. (1994)	$1.04 \cdot 10^{-5}$	Fuller et al. (1966)

(a) in M atm^{-1}; (b) in K; (c) in m^2 s^{-1}

Table S4 Implemented aqueous-phase reactions in the CAPRAM-DM1.0red

② reactions that run in the cloud mode 'sub#1', ③ reactions that run in the aerosol mode 'sub#2'

Nr.	Reaction	Rate constant(a)	Reference
D38	$DMS + O_3 \rightarrow DMSO + O_2$	$k = 8.61\cdot10^{+08}\exp(-2600/T)$	Gershenzon et al. (2001)
D39	$DMSO + OH \rightarrow MSIA + CH_3$	$k = 6.65\cdot10^{+09}\exp(-1270/T)$	Zhu et al. (2003a)
D40③	$DMSO + SO_4^- \rightarrow MSIA + CH_3 + H^+ + SO_4^{2-}$	$k = 2.97\cdot10^{+09}\exp(-1440/T)$	Zhu et al. (2003b)
D41③	$DMSO + Cl_2^- \rightarrow MSIA + HCl + CH_3 + Cl^- - H_2O$	$k = 1.60\cdot10^{+07}$	Zhu (2004)
D42②	$MSIA + O_3 \rightarrow MSA + O_2$	$k = 3.50\cdot10^{+07}$	Herrmann and Zellner (1997)
D43	$MSI^- + OH \rightarrow CH_3 + 0.135\ SO_2 + 0.765\ MS^- + 0.765\ SO_3 - 0.765\ MSI^- + 0.9\ OH^- + 0.1\ HSO_3^-$	$k = 1.20\cdot10^{+10}$	Bardouki et al. (2002)
D44③	$MSI^- + Cl_2^- \rightarrow CH_3 + 0.15\ SO_2 + 0.85\ MS^- + 0.85\ SO_3 - 0.85\ MSI^- + 2\ Cl^-$	$k = 8.00\cdot10^{+08}$	Zhu et al. (2005)
D45②	$MSI^- + O_3 \rightarrow CH_3SO_3^- + O_2$	$k = 2.00\cdot10^{+06}$	Flyunt et al. (2001)
D46	$MS^- + OH \rightarrow HCHO + SO_3^- + H_2O – 0.5\ O_2$	$k = 1.29\cdot10^{+07}\exp(-2630/T)$	Zhu et al. (2003a)
D47②	$MS^- + Cl_2^- \rightarrow CH_3 + SO_3 + 2\ Cl^-$	$k = 3.89\cdot10^{+03}$	Zhu (2004)

(a) k^{2nd} in $l^3\ mol^{-1}\ s^{-1}$

Table S5 Implemented aqueous-phase equilibria in the CAPRAM-DM1.0red

② reactions that run in the cloud mode 'sub#1', ③ reactions that run in the aerosol mode 'sub#2'

	Equilibrium	K(a)	$k_{f,\,298}$(b)	E_A/R(c)	$k_{b,\,298}$(b)	E_A/R(c)	Reference
D48②	$MSIA \rightleftharpoons MSI^- + H^+$	$5.0\cdot10^{-03}$	$2.50\cdot10^{08}$		$5.00\cdot10^{10}$		Wudl et al. (1967)
D49②	$MSA \rightleftharpoons MS^- + H^+$	73	$3.65\cdot10^{12}$		$5.00\cdot10^{10}$		Clarke and Woodward (1966)

(a) in M^{m-n}, n order of reaction of forward reaction, m order of reaction of backward reaction; (b) k_{298}^{2nd} in $l^1\ mol^{-1}\ s^{-1}$, k_{298}^{1st} in s^{-1}; (c) in K

Table S6 Implemented gas-phase reactions in the CAPRAM-HM3.0red

Nr.	Reaction	Rate constant[(a)]	Comment
H1	$Cl + O_3 \rightarrow ClO$	$k = 2.80\cdot10^{-11}exp(-250/T)$	Atkinson et al. (2007)
H2	$ClO + HO_2 \rightarrow HOCl$	$k = 2.20\cdot10^{-12}exp(340/T)$	Atkinson et al. (2007)
H3	$HCl + OH \rightarrow Cl$	$k = 1.70\cdot10^{-12}exp(-230/T)$	Atkinson et al. (2007)
H4	$ClO + NO \rightarrow Cl + NO_2$	$k = 6.20\cdot10^{-12}exp(295/T)$	Atkinson et al. (2007)
H5	$Cl + NO_2 \rightarrow ClNO_2$	TROE	Sander et al. (2006)
H6	$ClO + NO_2 \rightarrow ClNO_3$	TROE	Atkinson et al. (2007)
H7	$ClNO_3 \rightarrow ClO + NO_2$	$k = [M]*2.75\cdot10^{-6}exp(11438/T)$	Anderson and Fahey (1990)
H8	$Cl + CH_4 \rightarrow CH_3O_2 + HCl$	$k = 6.60\cdot10^{-12}exp(-1240/T)$	IUPAC, Atkinson et al. (2006)
H9	$Cl + C_2H_6 \rightarrow C_2H_5O_2 + HCl$	$k = 8.30\cdot10^{-11}exp(-100/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H10	$Cl + C_3H_8 \rightarrow C_3H_7O_2 + HCl$	$k = 1.40\cdot10^{-10}$	IUPAC, Atkinson et al. (2006)
H11	Cl + BIGALKANE → ALKO2 + HCl	$k = 2.05\cdot10^{-10}$	IUPAC, Atkinson et al. (2006)
H12	$Cl + CH_3OH \rightarrow HCHO + HO_2 + HCl$	$k = 7.10\cdot10^{-11}exp(-75/T)$	IUPAC, Atkinson et al. (2006)
H13	$Cl + C_2H_5OH \rightarrow 0.92\ CH_3CHO + 0.92\ HO_2 + 0.08\ EO2 + HCl$	$k = 6.05\cdot10^{-11}exp(155/T)$	IUPAC, Atkinson et al. (2006)
H14	$Cl + ALKOH \rightarrow 1.25\ MEK + HO_2 + HCl$	$k = 2.70\cdot10^{-11}exp(525/T)$	IUPAC, Atkinson et al. (2006)
H15	$Cl + CH_3OOH \rightarrow HCl + 0.6\ CH_3O_2 + 0.4\ HCHO + 0.4\ OH$	$k = 5.90\cdot10^{-11}$	IUPAC, Atkinson et al. (2006)
H16	$Cl + C_2H_5OOH \rightarrow HCl + CH_3CHO + OH$	$k = 1.07\cdot10^{-10}$	Wallington et al. (1989)
H17	$ClO + CH_3O_2 \rightarrow Cl + O_2 + HCHO + HO_2$	$k = 1.80\cdot10^{-11}exp(-600/T)$	Burkholder et al. (2015)
H18	$Cl + HCHO \rightarrow HCl + CO + HO_2$	$k = 8.10\cdot10^{-11}exp(-34/T)$	IUPAC, Atkinson et al. (2006)
H19	$Cl + CH_3CHO \rightarrow HCl + CH_3CO_3$	$k = 8.00\cdot10^{-11}$	IUPAC, Atkinson et al. (2006)
H20	$Cl + C_2H_5CHO \rightarrow HCl + 1.5\ CH_3CO_3$	$k = 1.30\cdot10^{-10}$	IUPAC, Atkinson et al. (2006)
H21	$Cl + HYAC \rightarrow HCl + MGLY + HO_2$	$k = 5.70\cdot10^{-11}$	Orlando et al. (1999)
H22	$Cl + CH_3COCHO \rightarrow HCl + CH_3CO_3 + CO$	$k = 4.80\cdot10^{-11}$	Green et al. (1990)
H23	$Cl + GLYOXAL \rightarrow HCl + 2.0\ CO + HO_2$	$k = 3.80\cdot10^{-11}$	Niki et al. (1985)
H24	Cl + MEK → HCl + MEKO2	$k = 3.05\cdot10^{-11}exp(80/T)$	IUPAC, Atkinson et al. (2006)
H25	Cl + MACR → 0.2 MACRO2 + 0.8 CC(O[O])(CCl)C=O + 0.2 HCl	$k = 2.55\cdot10^{-10}$	Rate constant average Canosa-Mas et al. (2001), Wang et al. (2002), Orlando et al. (2003) & Kaiser et al. (2010),
H26	$CC(O[O])(CCl)C{=}O + HO_2 \rightarrow CH_3COCH_2Cl + CO + HO_2 + OH$	$k = 1.00\cdot10^{-11}$	Hasson et al. (2012)
H27	$CC(O[O])(CCl)C{=}O + NO \rightarrow CH_3COCH_2Cl + CO + HO_2 + NO_2$	$k = 1.17\cdot10^{-11}$	Hsin and Elrod (2007)

Nr.	Reaction	Rate constant[(a)]	Comment
H28	CC(O[O])(CCl)C=O + CH_3O_2 → CH_3COCH_2Cl + CO + HO_2 + HCHO	$k = 1.00 \cdot 10^{-12}$	Hasson et al. (2012)
H29	CC(O[O])(CCl)C=O + CH_3CO_3 → CH_3COCH_2Cl + CO + HO_2 + CH_3O_2	$k = 1.00 \cdot 10^{-11}$	estimated
H30	OH + CC(OO)(CCl)C=O → CH_3COCH_2Cl + CO + OH	$k = 3.77 \cdot 10^{-11}$	estimated
H31	Cl + MVK → CC(=O)C(O[O])CCl	$k = 2.10 \cdot 10^{-10}$	Canosa-Mas et al. (2001)
H32	CC(=O)C(O[O])CCl + HO_2 → CC(=O)C(OO)CCl	$k = 1.82 \cdot 10^{-13} \exp(1300/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H33	CC(=O)C(O[O])CCl + NO → $ClCH_2CHO$ + NO_2 + CH_3CO_3	$k = 2.70 \cdot 10^{-12} \exp(360/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H34	CC(=O)C(O[O])CCl+ NO_3 → $ClCH_2CHO$ + NO_2 + CH_3CO_3	$k = 2.30 \cdot 10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)
H35	CC(=O)C(O[O])CCl + CH_3O_2 → $ClCH_2CHO$ + CH_3CO_3 + HCHO	$k = 1.00 \cdot 10^{-12}$	estimated
H36	CC(=O)C(O[O])CCl + CH_3CO_3 → $ClCH_2CHO$ + CH_3CO_3 + CH_3O_2	$k = 1.00 \cdot 10^{-11}$	estimated
H37	OH + CC(=O)C(OO)CCl → $ClCH_2CHO$ + CH_3CO_3 + OH	$k = 3.95 \cdot 10^{-11}$	after MVKOOH in MCMv3.2, Rickard et al. (21.10.2013)
H38	Cl + BIGALD1 → MALO2 + HO_2 + HCl	$k = 1.35 \cdot 10^{-10}$	Martín et al. (2013)
H39	Cl + TOL → HCl + TOLO2	$k = 6.20 \cdot 10^{-11}$	Wang et al. (2005)
H40	Cl + XYL → HCl + XYLNO2	$k = 1.40 \cdot 10^{-10}$	Wang et al. (2005)
H41	Cl + BZALD → HCl + ACBZO2	$k = 1.00 \cdot 10^{-10}$	Thiault et al. (2002)
H42	Cl + GLYALD → HCl + $HOCH_2CO_3$	$k = 7.00 \cdot 10^{-11}$	Niki et al. (1987)
H43	Cl + CH_3COCH_3 → HCl + $CH_3COCH_2O_2$	$k = 3.20 \cdot 10^{-11} \exp(-815/T)$	Atkinson et al. (2006)
H44	Cl + C_2H_2 → 0.26 ClCHO + 0.21 Cl + 0.53 HCl + 0.21 GLYOXAL + 1.32 CO + 0.79 HO_2	TROE	Atkinson et al. (2006)
H45	Cl + C_2H_4 → $ClCH_2CH_2O_2$	TROE	Atkinson et al. (2006)
H46	$ClCH_2CH_2O_2$ + HO_2 → $ClCH_2CH_2OOH$	$k = 3.30 \cdot 10^{-13} \exp(820/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H47	$ClCH_2CH_2O_2$ + NO → $ClCH_2CHO$ + HO_2 + NO_2	$k = 3.24 \cdot 10^{-12} \exp(360/T)$	Atkinson et al. (2008)
H48	$ClCH_2CH_2O_2$ + NO_3 → $ClCH_2CHO$ + HO_2 + NO_2	$k = 2.30 \cdot 10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)
H49	$ClCH_2CH_2O_2$ + CH_3O_2 → $ClCH_2CHO$ + 0.8 HCHO + 0.2 CH_3OH + 1.4 HO_2	$k = 2.00 \cdot 10^{-12}$	estimated
H50	$ClCH_2CHO$ + NO_3 → $ClCH_2CO_3$ + HNO_3	$k = 1.40 \cdot 10^{-12} \exp(-1860/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H51	$ClCH_2CHO$ + OH → $ClCH_2CO_3$ + H_2O	$k = 2.09 \cdot 10^{-11}$	Atkinson et al. (2008)
H52	$ClCH_2CO_3$ + HO_2 → 0.44 $ClCH_2O_2$ + 0.44 OH + 0.15 $ClCH_2COOH$ + 0.15 O_3 + 0.41 $ClCH_2C(O)OOH$	$k = 5.20 \cdot 10^{-13} \exp(980/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H53	$ClCH_2CO_3$ + NO → $ClCH_2O_2$ + NO_2	$k = 7.50 \cdot 10^{-12} \exp(290/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H54	$ClCH_2CO_3$ + NO_2 → ClPAN	TROE	MCMv3.2, Rickard et al. (21.10.2013)
H55	$ClCH_2CO_3$ + NO_3 → $ClCH_2O_2$ + NO_2	$k = 4.00 \cdot 10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)

Nr.	Reaction	Rate constant[(a)]	Comment
H56	$ClCH_2CO_3 + CH_3O_2 \rightarrow 0.7\ ClCH_2O_2 + 0.3\ ClCH_2COOH + 0.7\ HO_2 + HCHO$	$k = 1.00 \cdot 10^{-11}$	estimated
H57	$ClCH_2COOH + OH \rightarrow ClCH_2O_2$	$k = 1.90 \cdot 10^{-12} exp(190/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H58	$ClCH_2C(O)OOH + OH \rightarrow ClCH_2O_2$	$k = 4.29 \cdot 10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)
H59	$ClPAN + OH \rightarrow ClCHO + CO + NO_2$	$k = 6.26 \cdot 10^{-13}$	MCMv3.2, Rickard et al. (21.10.2013)
H60	$ClPAN \rightarrow ClCH_2CO_3 + NO_2$	TROE	MCMv3.2, Rickard et al. (21.10.2013)
H61	$ClCH_2O_2 + HO_2 \rightarrow 0.3\ ClCH_2OOH + 0.7\ ClCHO$	$k = 3.20 \cdot 10^{-13} exp(820/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H62	$ClCH_2O_2 + NO \rightarrow ClCHO + HO_2 + NO_2$	$k = 4.05 \cdot 10^{-12} exp(360/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H63	$ClCH_2O_2 + NO_3 \rightarrow ClCHO + HO_2 + NO_2$	$k = 2.30 \cdot 10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)
H64	$ClCH_2O_2 + CH_3O_2 \rightarrow 1.4\ HO_2 + ClCHO + 0.8\ HCHO + 0.2\ CH_3OH$	$k = 2.50 \cdot 10^{-12}$	estimated
H65	$Cl + C_3H_6 \rightarrow 0.4\ CH_3CH(O_2)CH_2Cl + 0.5\ CH_3CH(Cl)CH_2O_2 + 0.1\ HYAC$	$k = 1.43 \cdot 10^{-14} exp(2886/T)$	Atkinson et al. (2006)
H66	$CH_3CH(O_2)CH_2Cl + NO \rightarrow CH_3COCH_2Cl + HO_2 + NO_2$	$k = 2.70 \cdot 10^{-12} exp(360/T)$	Atkinson et al. (2008)
H67	$CH_3CH(Cl)CH_2O_2 + NO \rightarrow CH_3CH(Cl)CHO + NO_2 + HO_2$	$k = 2.70 \cdot 10^{-12} exp(360/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H68	$CH_3CH(O_2)CH_2Cl + CH_3O_2 \rightarrow CH_3COCH_2Cl + 0.8\ HCHO + 0.2\ CH_3OH + 1.4\ HO_2$	$k = 4.00 \cdot 10^{-14}$	estimated
H69	$CH_3CH(Cl)CH_2O_2 + CH_3O_2 \rightarrow CH_3CH(Cl)CHO + 0.8\ HCHO + 0.2\ CH_3OH + 1.4\ HO_2$	$k = 6.48 \cdot 10^{-13}$	estimated
H70	$CH_3COCH_2Cl + OH \rightarrow CH_3COCHClO_2$	$k = 3.68 \cdot 10^{-13}$	Atkinson et al. (2008)
H71	$CH_3COCHClO_2 + HO_2 \rightarrow CH_3COCHClOOH$	$k = 3.30 \cdot 10^{-13} exp(820/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H72	$CH_3COCHClO_2 + NO \rightarrow ClCHO + CH_3CO_3 + NO_2$	$k = 2.70 \cdot 10^{-12} exp(360/T)$	Atkinson et al. (2008)
H73	$CH_3COCHClO_2 + NO_3 \rightarrow ClCHO + CH_3CO_3 + NO_2$	$k = 2.30 \cdot 10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)
H74	$CH_3COCHClO_2 + CH_3O_2 \rightarrow ClCHO + CH_3CO_3 + 0.8\ HCHO + 0.2\ CH_3OH + HO_2$	$k = 2.00 \cdot 10^{-12}$	estimated
H75	$CH_3COCHClOOH + OH \rightarrow CH_3COCHClO_2$	$k = 8.34 \cdot 10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)
H76	$ClCHO + NO_3 \rightarrow CO + Cl + HNO_3$	$k = 1.40 \cdot 10^{-12} exp(-1860/T)$	Atkinson et al. (2008)
H77	$ClCHO + OH \rightarrow CO + Cl + H_2O$	$k = 6.12 \cdot 10^{-12}$	Atkinson et al. (2008)
H78	$CH_3CH(Cl)CHO + OH \rightarrow CH_3CH(Cl)C(O)O_2$	$k = 4.90 \cdot 10^{-12} exp(405/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H79	$CH_3CH(Cl)CHO + NO_3 \rightarrow CH_3CH(Cl)C(O)O_2 + HNO_3$	$k = 3.24 \cdot 10^{-12} exp(-1860/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H80	$CH_3CH(Cl)C(O)O_2 + HO_2 \rightarrow 0.15\ CH_3CH(Cl)COOH + 0.15\ O_3 + 0.41\ CH_3CH(Cl)C(O)OOH + 0.44\ CH_3CH(Cl)O_2 + 0.44\ OH$	$k = 5.20 \cdot 10^{-13} exp(980/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H81	$CH_3CH(Cl)C(O)O_2 + NO \rightarrow CH_3CH(Cl)O_2 + NO_2$	$k = 7.50 \cdot 10^{-12} exp(290/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H82	$CH_3CH(Cl)CO_3 + NO_2 \rightarrow CH_3ClPAN$	TROE	MCMv3.2, Rickard et al. (21.10.2013)

Nr.	Reaction	Rate constant[(a)]	Comment
H83	$CH_3ClPAN \rightarrow CH_3CH(Cl)CO_3 + NO_2$	TROE	MCMv3.2, Rickard et al. (21.10.2013)
H84	$CH_3CH(Cl)C(O)O_2 + NO_3 \rightarrow CH_3CH(Cl)O_2 + NO_2$	$k = 4.00\cdot10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)
H85	$CH_3CH(Cl)C(O)O_2 + CH_3O_2 \rightarrow 0.3\ CH_3CH(Cl)COOH + 0.7\ CH_3CH(Cl)O_2 + HCHO + HO_2$	$k = 1.00\cdot10^{-11}$	estimated
H86	CC(Cl)C(=O)OO + OH → CC(Cl)C(=O)O[O]	$k = 4.42\cdot10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)
H87	$CH_3CH(Cl)COOH + OH \rightarrow CH_3CH(Cl)O_2$	$k = 1.20\cdot10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)
H88	$CH_3CH(Cl)O_2 + HO_2 \rightarrow CH_3CH(Cl)OOH$	$k = 3.30\cdot10^{-13}exp(820/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H89	$CH_3CH(Cl)O_2 + NO \rightarrow CH_3CHO + Cl + NO_2$	$k = 4.05\cdot10^{-12}exp(360/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H90	$CH_3CH(Cl)O_2 + NO_3 \rightarrow CH_3CHO + Cl + NO_2$	$k = 2.30\cdot10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)
H91	$CH_3CH(Cl)O_2 + CH_3O_2 \rightarrow 0.6\ CH_3CHO + 0.6\ Cl + 0.4\ CH_3C(O)Cl + 0.8\ HCHO + 0.2\ CH_3OH + 0.8\ HO_2$	$k = 2.65\cdot10^{-12}$	estimated
H92	$CH_3CH(Cl)OOH + OH \rightarrow CH_3CH(Cl)O_2 + H_2O$	$k = 1.90\cdot10^{-12}exp(190/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H93	$CH_3CH(Cl)OOH + OH \rightarrow CH_3C(O)Cl + OH + H_2O$	$k = 9.95\cdot10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)
H94	$CH_3C(O)Cl + OH \rightarrow ClCOCH_2O_2 + H_2O$	$k = 3.88\cdot10^{-14}$	MCMv3.2, Rickard et al. (21.10.2013)
H95	$ClCOCH_2O_2 + HO_2 \rightarrow ClCOCH_2OOH$	$k = 3.30\cdot10^{-13}exp(820/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H96	$ClCOCH_2O_2 + NO \rightarrow HCHO + Cl + CO + NO_2$	$k = 3.24\cdot10^{-12}exp(360/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H97	$ClCOCH_2O_2 + NO_3 \rightarrow HCHO + Cl + CO + NO_2$	$k = 2.30\cdot10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)
H98	$ClCOCH_2O_2 + CH_3O_2 \rightarrow 2\ HCHO + Cl + CO + HO_2$	$k = 2.00\cdot10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)
H99	$Br + O_3 \rightarrow BrO$	$k = 1.70\cdot10^{-11}exp(-800/T)$	Atkinson et al. (2007)
H100	$BrO + HO_2 \rightarrow HOBr$	$k = 4.50\cdot10^{-12}exp(-500/T)$	Atkinson et al. (2007)
H101	$BrO + BrO \rightarrow 1.7\ Br + 0.15\ Br_2$	$k = 1.60\cdot10^{-12}exp(-210/T)$	Atkinson et al. (2007)
H102	$Br + NO_2 \rightarrow BrNO_2$	TROE	Atkinson et al. (2007)
H103	$BrO + NO \rightarrow Br + NO_2$	$k = 8.70\cdot10^{-12}exp(-260/T)$	Atkinson et al. (2007)
H104	$BrO + NO_2 \rightarrow BrNO_3$	TROE	Atkinson et al. (2007)
H105	$BrNO_3 \rightarrow BrO + NO_2$	$k = 2.79\cdot10^{13}exp(-12360/T)$	Orlando and Tyndall (1996)
H106	$Br + BrNO_3 \rightarrow Br_2 + NO_3$	$k = 4.90\cdot10^{-11}$	Orlando and Tyndall (1996)
H107	$BrO + ClO \rightarrow 0.95\ Br + 0.5\ OClO + 0.45\ Cl + 0.05\ BrCl$	$k = 7.32\cdot10^{-12}exp(-200/T)$	Summation A-Factor Burkholder et al. (2015)
H108	$BrO + CH_3O_2 \rightarrow 0.25\ Br + 0.25\ HCHO + 0.25\ HO_2 + 0.75\ HOBr + 0.75\ HCOOH$	$k = 4.10\cdot10^{-13}exp(-800/T)$	Bräuer et al. (2013)
H109	$Br + C_2H_2 \rightarrow 0.17\ BrCHO + 0.09\ Br + 0.74\ HBr + 0.09$ GLYOXAL $+ 1.65\ CO + 0.91\ HO_2$	$k = 6.35\cdot10^{-15}exp(-440/T)$	Atkinson et al. (2006)

Nr.	Reaction	Rate constant[(a)]	Comment
H110	$Br + HCHO \rightarrow HBr + CO + HO_2$	$k = 1.70\cdot10^{-11}exp(-800/T)$	Sander et al. (2006)
H111	$BrO + HCHO \rightarrow HOBr + CO + HO_2$	$k = 1.50\cdot10^{-14}$	Hansen et al. (1999)
H112	$Br + CH_3CHO \rightarrow HBr + CH_3CO_3$	$k = 1.80\cdot10^{-11}exp(-460/T)$	Atkinson et al. (2006)
H113	$Br + C_2H_5CHO \rightarrow HBr + 1.5\ CH_3CO_3$	$k = 5.75\cdot10^{-11}exp(-610/T)$	Ramacher et al. (2000)
H114	$Br + C_2H_4 \rightarrow BrCH_2CH_2O_2$	$k = 2.25\cdot10^{-13}exp(-277/T)$	Atkinson et al. (2006)
H115	$BrCH_2CH_2O_2 + NO \rightarrow BrCH_2CHO + HO_2 + NO_2$	$k = 9.70\cdot10^{-12}$	Atkinson et al. (2008)
H116	$BrCH_2CH_2O_2 + CH_3O_2 \rightarrow BrCH_2CHO + 0.8\ HCHO + 0.2\ CH_3OH + 1.4\ HO_2$	$k = 2.00\cdot10^{-12}$	Bräuer et al. (2013)
H117	$BrCH_2CHO + OH \rightarrow BrCH_2CO_3 + H_2O$	$k = 2.05\cdot10^{-12}$	Atkinson et al. (2008)
H118	$BrCH_2CO_3 + HO_2 \rightarrow 0.15\ BrCH_2COOH + 0.15\ O_3 + 0.41\ BrCH_2C(O)OOH + 0.44\ BrCH_2O_2 + 0.44\ OH$	$k = 5.20\cdot10^{-13}exp(980/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H119	$BrCH_2CO_3 + NO \rightarrow BrCH_2O_2 + NO_2$	$k = 7.50\cdot10^{-12}exp(290/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H120	$BrCH_2CO_3 + CH_3O_2 \rightarrow 0.7\ BrCH_2O_2 + 0.3\ BrCH_2COOH + 0.7\ HO_2 + HCHO$	$k = 1.00\cdot10^{-11}$	Bräuer et al. (2013)
H121	$BrCH_2COOH + OH \rightarrow BrCH_2O_2 + H_2O$	$k = 1.90\cdot10^{-12}exp(190/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H122	$BrCH_2C(O)OOH + OH \rightarrow BrCH_2CO_3 + H_2O$	$k = 3.79\cdot10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)
H123	$BrCH_2O_2 + HO_2 \rightarrow BrCH_2OOH$	$k = 4.28\cdot10^{-13}exp(820/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H124	$BrCH_2O_2 + NO \rightarrow BrCHO + HO_2 + NO_2$	$k = 4.05\cdot10^{-12}exp(360/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H125	$BrCH_2O_2 + NO_3 \rightarrow BrCHO + HO_2 + NO_2$	$k = 2.30\cdot10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)
H126	$BrCH_2O_2 + CH_3O_2 \rightarrow 1.4\ HO_2 + BrCHO + 0.8\ HCHO + 0.2\ CH_3OH$	$k = 2.00\cdot10^{-12}$	Bräuer et al. (2013)
H127	$BrCH_2OOH + OH \rightarrow BrCH_2O_2 + H_2O$	$k = 1.90\cdot10^{-12}exp(190/T)$	MCMv3.2, Rickard et al. (21.10.2013)
H128	$BrCH_2OOH + OH \rightarrow BrCHO + OH + H_2O$	$k = 5.79\cdot10^{-12}$	MCMv3.2, Rickard et al. (21.10.2013)
H129	$BrCHO + NO_3 \rightarrow CO + Br + HNO_3$	$k = 1.40\cdot10^{-12}exp(-1860/T)$	Atkinson et al. (2008)
H130	$BrCHO + OH \rightarrow CO + Br + H_2O$	$k = 1.16\cdot10^{-12}$	Atkinson et al. (2008)
H131	$Br + C_3H_6 \rightarrow CH_3CH(O_2)CH_2Br$	$k = 3.60\cdot10^{-12}$	Atkinson et al. (2006)
H132	$CH_3CH(O_2)CH_2Br + NO \rightarrow CH_3COCH_2Br + HO_2 + NO_2$	$k = 2.70\cdot10^{-12}exp(360/T)$	Atkinson et al. (2008)
H133	$CH_3CH(O_2)CH_2Br + CH_3O_2 \rightarrow CH_3COCH_2Br + 0.8\ HCHO + 0.2\ CH_3OH + 1.4\ HO_2$	$k = 4.00\cdot10^{-14}$	Bräuer et al. (2013)
H134	$CH_3COCH_2Br + OH \rightarrow CH_3COCHBrO_2$	$k = 8.80\cdot10^{-12}exp(-1320/T)$	Atkinson et al. (2008)
H135	$CH_3COCHBrO_2 + NO \rightarrow CH_3CO_3 + BrCHO + NO_2$	$k = 8.00\cdot10^{-12}$	Atkinson et al. (2008)
H136	$CH_3COCHBrO_2 + CH_3O_2 \rightarrow 0.4\ CH_3COC(O)Br + 0.6\ CH_3CO_3 + 0.6\ BrCHO + 0.8\ HO_2 + 0.8\ HCHO + 0.2\ CH_3OH$	$k = 2.00\cdot10^{-12}$	Bräuer et al. (2013)

Nr.	Reaction	Rate constant[(a)]	Comment
H137	$I + O_3 \rightarrow IO$	$k = 2.10 \cdot 10^{-11} exp(-830/T)$	Atkinson et al. (2007)
H138	$I_2 + OH \rightarrow I + HOI$	$k = 2.10 \cdot 10^{-10}$	Atkinson et al. (2007)
H139	$IO + HO_2 \rightarrow HOI$	$k = 1.40 \cdot 10^{-11} exp(540/T)$	Atkinson et al. (2007)
H140	$IO + IO \rightarrow 0.38\ OIO + 0.46\ I_2O_2 + 0.6\ I + 0.05\ I_2$	$k = 5.40 \cdot 10^{-11} exp(180/T)$	Sander et al. (2006)
H141	$OIO + OH \rightarrow HIO_3$	$k = 2.20 \cdot 10^{-10} exp(243/T)$	von Glasow et al. (2002)
H142	$IO + O_3 \rightarrow 0.83\ I + 0.17\ OIO$	$k = 1.20 \cdot 10^{-15}$	(Larin et al., 1999)
H143	$IO + OIO \rightarrow I_2O_3$	$k = 1.00 \cdot 10^{-10}$	(Gómez Martín et al., 2007)
H144	$I_2O_3 \rightarrow IO + OIO$	$k = 2.78 \cdot 10^{-11}$	(Kaltsoyannis and Plane, 2008)
H145	$OIO + OIO \rightarrow I_2O_4$	$k = 1.00 \cdot 10^{-10}$	(Saunders and Plane, 2005)
H146	$I_2O_4 \rightarrow OIO + OIO$	$k = 1.67 \cdot 10^{+00}$	(Kaltsoyannis and Plane, 2008)
H147	$I_2 + O_3 \rightarrow IO + I$	$k = 4.02 \cdot 10^{-15} exp(-2050/T)$	(Vikis and Macfarlane, 1985)
H148	$I_2O_2 \rightarrow 0.995\ OIO + 0.995\ I + 0.01\ IO$	$k = 1.00 \cdot 10^{+01}$	(Kaltsoyannis and Plane, 2008)
H149	$I_2 + NO_3 \rightarrow I + INO_3$	$k = 1.50 \cdot 10^{-12}$	Atkinson et al. (2007)
H150	$IO + NO \rightarrow I + NO_2$	$k = 7.15 \cdot 10^{-12} exp(300/T)$	Atkinson et al. (2007)
H151	$IO + NO_2 \rightarrow INO_3$	TROE	Atkinson et al. (2007)
H152	$INO_3 \rightarrow IO + NO_2$	$k = [M]*4.40 \cdot 10^{-05} exp(12060/T)$	Atkinson et al. (2007)
H153	$IO + CH_3O_2 \rightarrow I + HO_2 + HCHO$	$k = 2.00 \cdot 10^{-12}$	(Dillon et al., 2006)
H154	$IO + ClO \rightarrow 0.8\ I + 0.55\ OClO + 0.25\ Cl + 0.2\ ICl$	$k = 4.70 \cdot 10^{-12} exp(280/T)$	Atkinson et al. (2007)
H155	$IO + BrO \rightarrow 0.8\ OIO + Br + 0.2\ I$	$k = 1.50 \cdot 10^{-11} exp(510/T)$	Atkinson et al. (2007)
Photolysis reactions			
H156	$Cl_2 \rightarrow Cl + Cl$	$J = 3.827 \cdot 10^{-03} cos(\chi)^{0.543} exp(-0.244/cos(\chi))$	Bräuer et al. (2013)
H157	$ClO \rightarrow Cl + O(^3P)$	$J = 4.755 \cdot 10^{-04} cos(\chi)^{1.258} exp(-0.588/cos(\chi))$	Bräuer et al. (2013)
H158	$OClO \rightarrow ClO + O(^3P)$	$J = 1.332 \cdot 10^{-01} cos(\chi)^{0.416} exp(-0.244/cos(\chi))$	Bräuer et al. (2013)
H159	$HOCl \rightarrow Cl + OH$	$J = 4.615 \cdot 10^{-04} cos(\chi)^{0.656} exp(-0.240/cos(\chi))$	Bräuer et al. (2013)
H160	$ClNO_2 \rightarrow Cl + NO_2$	$J = 6.219 \cdot 10^{-04} cos(\chi)^{0.774} exp(-0.255/cos(\chi))$	Bräuer et al. (2013)
H161	$ClNO_3 \rightarrow Cl + NO_3$	$J = 6.420 \cdot 10^{-05} cos(\chi)^{0.648} exp(-0.217/cos(\chi))$	Bräuer et al. (2013)
H162	$ClNO_3 \rightarrow ClO + NO_2$	$J = 1.393 \cdot 10^{-05} cos(\chi)^{1.052} exp(-0.243/cos(\chi))$	Bräuer et al. (2013)
H163	$CC(=O)C(OO)CCl \rightarrow ClCH_2CHO + CH_3CO_3 + OH$	$J = 7.649 \cdot 10^{-05} cos(\chi)^{0.682} exp(-0.279/cos(\chi))$	Bräuer et al. (2013)
H164	$ClCH_2CH_2OOH \rightarrow ClCH_2CHO + HO_2 + OH$	$J = 7.649 \cdot 10^{-06} cos(\chi)^{0.682} exp(-0.279/cos(\chi))$	Bräuer et al. (2013)
H165	$ClCH_2CHO \rightarrow ClCH_2O_2 + HO_2 + CO$	$J = 4.642 \cdot 10^{-05} cos(\chi)^{0.762} exp(-0.353/cos(\chi))$	Bräuer et al. (2013)

Nr.	Reaction	Rate constant[(a)]	Comment
H166	$ClCH_2C(O)OOH \rightarrow ClCH_2O_2 + OH$	$J = 7.649\cdot10^{-06}\cos(\chi)^{0.682}\exp(-0.279/\cos(\chi))$	Bräuer et al. (2013)
H167	$ClCH_2OOH \rightarrow ClCHO + HO_2 + OH$	$J = 7.649\cdot10^{-06}\cos(\chi)^{0.682}\exp(-0.279/\cos(\chi))$	Bräuer et al. (2013)
H168	$CH_3CH(O)CH_2Cl \rightarrow CH_3O_2 + ClCH_2CO_3$	$J = 5.804\cdot10^{-06}\cos(\chi)^{1.092}\exp(-0.377/\cos(\chi))$	Bräuer et al. (2013)
H169	$CH_3CH(O)CHClOOH \rightarrow ClCHO + CH_3CO_3 + OH$	$J = 7.649\cdot10^{-06}\cos(\chi)^{0.682}\exp(-0.279/\cos(\chi))$	Bräuer et al. (2013)
H170	$ClCHO \rightarrow HO_2 + CO + Cl$	$J = 4.642\cdot10^{-05}\cos(\chi)^{0.762}\exp(-0.353/\cos(\chi))$	Bräuer et al. (2013)
H171	$CH_3CH(Cl)CHO \rightarrow CH_3CH(Cl)O_2 + HO_2 + CO$	$J = 2.879\cdot10^{-05}\cos(\chi)^{1.067}\exp(-0.358/\cos(\chi))$	Bräuer et al. (2013)
H172	$CH_3CH(Cl)OOH \rightarrow CH_3CHO + Cl + OH$	$J = 7.649\cdot10^{-06}\cos(\chi)^{0.682}\exp(-0.279/\cos(\chi))$	Bräuer et al. (2013)
H173	$CH_3C(O)Cl \rightarrow CH_3CO_3 + Cl$	$J = 5.804\cdot10^{-06}\cos(\chi)^{1.092}\exp(-0.377/\cos(\chi))$	Bräuer et al. (2013)
H174	$ClCOCH_2OOH \rightarrow ClCOCH_2O_2 + OH$	$J = 7.649\cdot10^{-06}\cos(\chi)^{0.682}\exp(-0.279/\cos(\chi))$	Bräuer et al. (2013)
H175	$Br_2 \rightarrow Br + Br$	$J = 4.773\cdot10^{-02}\cos(\chi)^{0.193}\exp(-0.213/\cos(\chi))$	Bräuer et al. (2013)
H176	$BrO \rightarrow Br + O(^3P)$	$J = 6.368\cdot10^{-02}\cos(\chi)^{0.605}\exp(-0.269/\cos(\chi))$	Bräuer et al. (2013)
H177	$HOBr \rightarrow Br + OH$	$J = 3.464\cdot10^{-03}\cos(\chi)^{0.441}\exp(-0.214/\cos(\chi))$	Bräuer et al. (2013)
H178	$BrNO_2 \rightarrow Br + NO_2$	$J = 7.443\cdot10^{-03}\cos(\chi)^{0.355}\exp(-0.236/\cos(\chi))$	Bräuer et al. (2013)
H179	$BrNO_3 \rightarrow 0.29\ Br + 0.29\ NO_3 + 0.71\ BrO + 0.71\ NO_2$	$J = 2.194\cdot10^{-04}\cos(\chi)^{0.492}\exp(-0.215/\cos(\chi))$	Bräuer et al. (2013)
H180	$BrCl \rightarrow Br + Cl$	$J = 1.650\cdot10^{-02}\cos(\chi)^{0.297}\exp(-0.224/\cos(\chi))$	Bräuer et al. (2013)
H181	$BrCH_2CHO \rightarrow BrCH_2O_2 + HO_2 + CO$	$J = 4.642\cdot10^{-05}\cos(\chi)^{0.762}\exp(-0.353/\cos(\chi))$	Bräuer et al. (2013)
H182	$BrCH_2C(O)OOH \rightarrow BrCH_2O_2 + OH$	$J = 7.649\cdot10^{-06}\cos(\chi)^{0.682}\exp(-0.279/\cos(\chi))$	Bräuer et al. (2013)
H183	$BrCH_2OOH \rightarrow BrCHO + OH + HO_2$	$J = 7.649\cdot10^{-06}\cos(\chi)^{0.682}\exp(-0.279/\cos(\chi))$	Bräuer et al. (2013)
H184	$BrCHO \rightarrow HO_2 + CO + Br$	$J = 4.642\cdot10^{-05}\cos(\chi)^{0.762}\exp(-0.353/\cos(\chi))$	Bräuer et al. (2013)
H185	$CH_3COCH_2Br \rightarrow 0.7\ CO + 0.7\ Br + 0.7\ CH_3CO_3 + 0.3\ BrCH_2CO_3 + 0.3\ CH_3O_2$	$J = 3.523\cdot10^{-04}\cos(\chi)^{0.885}\exp(-0.283/\cos(\chi))$	Bräuer et al. (2013)
H186	$CH_3COC(O)Br \rightarrow CO + Br + CH_3CO_3$	$J = 1.853\cdot10^{-04}\cos(\chi)^{0.583}\exp(-0.225/\cos(\chi))$	Bräuer et al. (2013)
H187	$CHBr_3 \rightarrow 3\ Br + CO + HO_2$	$J = 2.228\cdot10^{-06}\cos(\chi)^{1.471}\exp(-0.230/\cos(\chi))$	Bräuer et al. (2013)
H188	$I_2 \rightarrow I + I$	$J = 2.165\cdot10^{-01}\cos(\chi)^{0.125}\exp(-0.185/\cos(\chi))$	Bräuer et al. (2013)
H189	$IO \rightarrow I + O(^3P)$	$J = 2.640\cdot10^{-03}\cos(\chi)^{0.240}\exp(-0.240/\cos(\chi))$	Bräuer et al. (2013)
H190	$OIO \rightarrow 0.96\ I + 0.04\ IO + 0.04\ O(^3P)$	$J = 4.054\cdot10^{-02}\cos(\chi)^{0.119}\exp(-0.185/\cos(\chi))$	Bräuer et al. (2013)
H191	$HOI \rightarrow I + OH$	$J = 1.469\cdot10^{-02}\cos(\chi)^{0.342}\exp(-0.236/\cos(\chi))$	Bräuer et al. (2013)
H192	$INO_3 \rightarrow 0.85\ I + 0.85\ NO_3 + 0.15\ IO + 0.15\ NO_2$	$J = 6.599\cdot10^{-02}\cos(\chi)^{0.530}\exp(-0.243/\cos(\chi))$	Bräuer et al. (2013)
H193	$ICl \rightarrow I + Cl$	$J = 3.403\cdot10^{-02}\cos(\chi)^{0.179}\exp(-0.207/\cos(\chi))$	Bräuer et al. (2013)
H194	$IBr \rightarrow I + Br$	$J = 1.000\cdot10^{-01}\cos(\chi)^{0.149}\exp(-0.197/\cos(\chi))$	Bräuer et al. (2013)
H195	$C_3H_7I \rightarrow I + C_3H_7O_2$	$J = 3.731\cdot10^{-05}\cos(\chi)^{1.292}\exp(-0.217/\cos(\chi))$	Bräuer et al. (2013)
H196	$CH_2I_2 \rightarrow 2\ I + 2\ HO_2$	$J = 1.496\cdot10^{-02}\cos(\chi)^{0.801}\exp(-0.265/\cos(\chi))$	Bräuer et al. (2013)

Nr.	Reaction	Rate constant(a)	Comment
H197	$CH_3I \rightarrow I + CH_3O_2$	$J = 1.206\cdot10^{-05}\cos(\chi)^{1.254}\exp(-0.231/\cos(\chi))$	Bräuer et al. (2013)
H198	$ClCH_2I \rightarrow I + ClCH_2O_2$	$J = 6.910\cdot10^{-04}\cos(\chi)^{1.057}\exp(-0.238/\cos(\chi))$	Bräuer et al. (2013)
H199	$BrCH_2I \rightarrow I + BrCH_2O_2$	$J = 4.261\cdot10^{-04}\cos(\chi)^{0.976}\exp(-0.250/\cos(\chi))$	Bräuer et al. (2013)

(a) k^{2nd} in cm^3 $molecules^{-1}$ s^{-1}; k^{1st} in s^{-1}; J in s^{-1}

Table S7 Parameters for pressure dependent reactions.

	Reaction	TYPE	k_0(a)	k_∞(a)	F_C
H5	$Cl + NO_2 \rightarrow ClNO_2$	TROE	$1.80\cdot10^{-31}*(T/298)^{-2.0}$	$1.00\cdot10^{-10}*(T/298)^{-1.0}$	0.6
H6	$ClO + NO_2 \rightarrow ClNO_3$	TROE	$1.60\cdot10^{-31}*(T/298)^{-3.4}$	$7.00\cdot10^{-11}$	0.4
H44	$Cl + C_2H_2 \rightarrow 0.26\ ClCHO + 0.21\ Cl + 0.53\ HCl + 0.21$ GLYOXAL $+ 1.32\ CO + 0.79\ HO_2$	TROE	$6.10\cdot10^{-30}*(T/298)^{-3.0}$	$2.00\cdot10^{-10}$	0.6
H45	$Cl + C_2H_4 \rightarrow ClCH_2CH_2O_2$	TROE	$1.85\cdot10^{-29}*(T/298)^{-3.3}$	$6.00\cdot10^{-10}$	0.4
H54	$ClCH_2CO_3 + NO_2 \rightarrow$ ClPAN	TROE	$2.70\cdot10^{-28}*(T/298)^{7.1}$	$1.20\cdot10^{-11}*(T/298)^{0.9}$	0.3
H60	ClPAN $\rightarrow ClCH_2CO_3 + NO_2$	TROE	$4.90\cdot10^{-03}\exp(-12100/T)$	$5.40\cdot10^{+16}\exp(-13830/T)$	0.3
H82	$CH_3CH(Cl)CO_3 + NO_2 \rightarrow CH_3$ClPAN	TROE	$2.70\cdot10^{-28}*(T/298)^{7.1}$	$1.20\cdot10^{-11}*(T/298)^{0.9}$	0.3
H83	CH_3ClPAN $\rightarrow CH_3CH(Cl)CO_3 + NO_2$	TROE	$4.90\cdot10^{-03}\exp(-12100/T)$	$5.40\cdot10^{+16}\exp(-13830/T)$	0.3
H102	$Br + NO_2 \rightarrow BrNO_2$	TROE	$4.20\cdot10^{-31}*(T/298)^{-2.4}$	$2.70\cdot10^{-11}$	0.55
H104	$BrO + NO_2 \rightarrow BrNO_3$	TROE	$4.70\cdot10^{-31}*(T/298)^{-3.1}$	$1.80\cdot10^{-11}$	0.4
H151	$IO + NO_2 \rightarrow INO_3$	TROE	$7.70\cdot10^{-31}(T/300)^{-5.0}$	$1.60\cdot10^{-11}$	0.6

(a) k^{2nd} in cm^3 $molecules^{-1}$ s^{-1}; k^{1st} in s^{-1}

Rate constants calculated with TROE formula: $k(T)= \frac{k_0(T)[M]}{1+\frac{k_0(T)[M]}{k_\infty(T)}} \times F_C^{\left\{1+log_{10}\left(\frac{k_0(T)[M]}{k_\infty(T)}\right)^2\right\}^{-1}}$

Table S8 Implemented phase transfers in the CAPRAM-HM3.0red

② reactions that run in the cloud mode 'sub#1', ③ reactions that run in the aerosol mode 'sub#2', ● already included in CAPRAM3.0red

	Species	$K_{H\ (298\ K)}$ (a)	$-\Delta H/R$ (b)	α	$D_{g\ (298\ K)}$ (c)	Comment
H200③●	Cl_2	$9.15\cdot10^{-2}$	2490	0.08	1.28	Bräuer et al. (2013)
H201	Cl	$2.00\cdot10^{-1}$		0.05	1.82	Bräuer et al. (2013)
H202②●	HCl	$1.10\cdot10^{0}$	2020	0.1026	1.89	Bräuer et al. (2013)
H203③	HOCl	$6.60\cdot10^{2}$	5862	0.5	1.51	Bräuer et al. (2013)
H204③●	$ClNO_2$	$2.40\cdot10^{-2}$		0.01	1.27	Bräuer et al. (2013)
H205③	$ClNO_3$	$2.10\cdot10^{5}$	8700	0.1	1.18	Bräuer et al. (2013)
H206	ClCHO	$3.00\cdot10^{3}$	7216	0.02	1.23	Bräuer et al. (2013)
H207③●	Br_2	$7.60\cdot10^{-1}$	4100	0.08	1.00	Bräuer et al. (2013)
H208	Br	$1.20\cdot10^{0}$		0.05	1.29	Bräuer et al. (2013)
H209③	HBr	$1.30\cdot10^{0}$	10239	0.0481	1.26	Bräuer et al. (2013)
H210③	HOBr	$9.30\cdot10^{1}$	5862	0.5	1.16	Bräuer et al. (2013)
H211③	$BrNO_3$	$2.10\cdot10^{5}$	8700	0.8	1.01	Bräuer et al. (2013)
H212③	BrCl	$9.40\cdot10^{-1}$	-5600	0.33	1.05	Bräuer et al. (2013)
H213	$BrCH_2CO_3$	$6.69\cdot10^{2}$	5893	0.019	0.84	Bräuer et al. (2013)
H214②	$BrCH_2COOH$	$1.52\cdot10^{5}$	9300	0.0322	0.84	Bräuer et al. (2013); Sander (2015)
H215	BrCHO	$7.40\cdot10^{1}$		0.02	1.02	Bräuer et al. (2013)
H216	I_2	$3.00\cdot10^{0}$	4431	0.0126	0.86	Bräuer et al. (2013)
H217③	HOI	$4.50\cdot10^{2}$	5862	0.5	1.08	Bräuer et al. (2013)
H218	HIO_3	$2.10\cdot10^{5}$	8700	0.0126	0.98	Bräuer et al. (2013)
H219③	INO_3	$2.10\cdot10^{5}$	8700	0.123	0.96	Bräuer et al. (2013)
H220③	I_2O_2	$1.00\cdot10^{4}$		0.123	0.80	Bräuer et al. (2013); Sander (2015)
H221③	ICl	$1.10\cdot10^{2}$	5600	0.0126	0.98	Bräuer et al. (2013)
H222③	IBr	$2.40\cdot10^{1}$	5600	0.0126	0.88	Bräuer et al. (2013)

(a) in $M\ atm^{-1}$; (b) in K; (c) in $m^2\ s^{-1}$

Table S9 Implemented aqueous-phase reactions in the CAPRAM-HM3.0red

② reactions that run in the cloud mode 'sub#1', ③ reactions that run in the aerosol mode 'sub#2', ● already included in CAPRAM3.0red

	Reaction	k_{298} (a)	E_A/R (b)	Comment
H223●	$Cl_2^- + H_2O_2 \rightarrow 2\ Cl^- + H^+ + HO_2$	$6.20\cdot10^{5}$	3340	Jacobi et al. (1999)
H224②●	$Cl_2^- + H_2O \rightarrow H^+ + Cl^- + ClOH^-$	$2.34\cdot10^{1}$		Buxton et al. (1998)
H225②	$HOCl + HO_2 \rightarrow Cl + H_2O + O_2$	$7.50\cdot10^{6}$		Bräuer et al. (2013)
H226	$HOCl + OH \rightarrow ClO + H_2O$	$2.00\cdot10^{9}$		Bräuer et al. (2013)
H227●	$Cl_2^- + HSO_3^- \rightarrow 2\ Cl^- + H^+ + SO_3^-$	$1.70\cdot10^{8}$	400	Jacobi (1996)
H228③	$HOCl + HSO_3^- \rightarrow Cl^- + H^+ + HSO_4^{2-}$	$7.60\cdot10^{8}$		Herrmann (2003)
H229	$Cl^- + HSO_5^- \rightarrow HOCl + SO_4^{2-}$	$1.80\cdot10^{-3}$	7352	Fortnum et al. (1960)
H230●	$Cl_2^- + Fe_2^+ \rightarrow 2\ Cl^- + Fe_3^+$	$1.00\cdot10^{7}$	3030	Thornton and Laurence (1973)
H231②●	$Cl^- + FeO_2^+ \rightarrow Fe_3^+ + ClOH^- + OH- - H_2O$	$1.00\cdot10^{2}$		Jacobsen et al. (1998)
H232●	$Cl_2^- + Mn_2^+ \rightarrow MnCl_2^+$	$2.00\cdot10^{7}$	4090	Laurence and Thornton (1973)
H233●	$MnCl_2^+ \rightarrow 0.588\ Cl_2^- + 0.588\ Mn^{2+} + 0.824\ Cl^- + 0.412\ Mn^{3+}$	$5.10\cdot10^{5}$		Deguillaume et al. (2010); Laurence and Thornton (1973)
H234	$2\ ClO \rightarrow Cl^- + ClO_3^- + 2\ H^+$	$2.50\cdot10^{9}$		Klaning and Wolff (1985)
H235	$OH + ClO_3^- \rightarrow ClO + O_2 + OH^-$	$1.00\cdot10^{6}$		Buxton and Subhani (1972)
H236	$Cl_2 + H_2O_2 \rightarrow 2\ H^+ + 2\ Cl^- + O_2$	$1.83\cdot10^{2}$	5387	Connick (1947)
H237③	$ClNO_3 \rightarrow HOCl + HNO_3$	$1.62\cdot10^{6}$	2800	Shi et al. (2001)
H238②	$Cl_2^- + HC_2O_4^- \rightarrow 2\ Cl^- + H^+ + C_2O_4^-$	$1.30\cdot10^{6}$		Bräuer et al. (2013)
H239②	$Cl_2^- + C_2O_4^{2-} \rightarrow 2\ Cl^- + C_2O_4^-$	$4.00\cdot10^{6}$		Bräuer et al. (2013)
H240②	$ClCHO \rightarrow CO + H^+ + Cl^-$	$1.00\cdot10^{4}$		Prager et al. (2001)
H241	$Br + H_2O_2 \rightarrow H^+ + Br^- + HO_2$	$4.00\cdot10^{9}$		Sutton et al. (1965)
H242②	$Br_2^- + HO_2 \rightarrow Br^- + 0.5\ Br_2 + 0.5\ H_2O_2 + 0.5\ O_2$	$8.80\cdot10^{9}$		Sutton and Downes (1972)
H243	$BrO + BrO \rightarrow BrO_2^- + HOBr + H^+$	$2.80\cdot10^{9}$		Klaning and Wolff (1985)
H244	$HOBr + OH \rightarrow BrO + H_2O$	$2.00\cdot10^{9}$		Klaning and Wolff (1985)
H245②	$HOBr + HO_2 \rightarrow Br + H_2O + O_2$	$1.00\cdot10^{9}$		Bräuer et al. (2013)
H246②	$HOBr + H_2O_2 \rightarrow H^+ + Br^- + H_2O + O_2$	$3.50\cdot10^{6}$		Young (1950)
H247③	$HOBr + HSO_3^- \rightarrow H+ + Br^- + HSO_4^-$	$5.00\cdot10^{9}$		Bräuer et al. (2013)
H248	$Br^- + HSO_5^- \rightarrow HOBr + SO_4^{2-}$	$1.00\cdot10^{0}$	5338	Fortnum et al. (1960)

② reactions that run in the cloud mode 'sub#1', ③ reactions that run in the aerosol mode 'sub#2', ● already included in CAPRAM3.0red				
	Reaction	**k_{298}(a)**	**E_A/R(b)**	**Comment**
H249	$Br^- + NO_3 \rightarrow Br + NO_3^-$	$3.80 \cdot 10^9$		Zellner et al. (1996)
H250	$Br_2^- + Fe^{2+} \rightarrow 2\ Br^- + Fe^{3+}$	$3.60 \cdot 10^6$	3330	Thornton and Laurence (1973)
H251●	$Br_2^- + Mn^{2+} \rightarrow MnBr_2^+$	$6.30 \cdot 10^6$	4330	Thornton and Laurence (1973)
H252●	$MnBr_2^+ \rightarrow 0.577\ Br_2^- + 0.577\ Mn^{2+} + 0.846\ Br^- + 0.423\ Mn^{3+}$	$5.20 \cdot 10^5$		Thornton and Laurence (1973); Deguillaume et al. (2010)
H253	$BrO_3^- + SO_4^- \rightarrow BrO + O_2 + SO_4^{2-}$	$1.40 \cdot 10^6$		Zuo and Katsumura (1998)
H254	$Br + O_3 \rightarrow BrO + O_2$	$1.50 \cdot 10^8$		Von Gunten and Oliveras (1998)
H255	$BrO_3^- + HSO_3^- \rightarrow BrO_2^- + SO_4^{2-} + H^+$	$2.70 \cdot 10^{-2}$		Szirovicza and Boga (1998)
H256	$BrO_3^- + OH \rightarrow BrO + O_2 + OH^-$	$5.00 \cdot 10^6$		Amichai et al. (1969)
H257③	$BrNO_3 \rightarrow HOBr + HNO_3$	$1.00 \cdot 10^9$		Hanson et al. (1996)
H258	$BrO_3^- + HC_2O_4^- \rightarrow BrO_2^- + 2\ CO_2 + H_2O$	$7.47 \cdot 10^{-4}$		Pelle et al. (2004)
H259②	$BrCHO \rightarrow CO + H^+ + Br^-$	$1.00 \cdot 10^4$		Bräuer et al. (2013)
H260②	$CH_2BrCO_3 + H_2O \rightarrow CH_2BrCOOH + HO_2$	$3.55 \cdot 10^5$		Bräuer et al. (2013)
H261	$Br_2^- + HCOO^- \rightarrow 2\ Br^- + COOH$	$4.90 \cdot 10^3$		Jacobi et al. (1996)
H262③	$Br^- + HOCl \rightarrow BrCl + H_2O - H^+$	$1.30 \cdot 10^6$		Kumar and Margerum (1987)
H263②	$BrO_2^- + HOCl \rightarrow 0.85\ ClO_3^- + 0.93\ HOBr + 0.08\ ClO_2^- + 0.07\ BrO_3^- + 0.92\ Cl^- + 0.92\ H^+ - 0.85\ HOCl$	$1.60 \cdot 10^2$		Nicoson et al. (2003)
H264	$I^- + O_3 \rightarrow HOI + O_2$	$2.17 \cdot 10^9$	8790	Magi et al. (1997)
H265②	$IO + IO \rightarrow HOI + HIO_3 + H^+ - H_2O - H_2O_2$	$1.50 \cdot 10^9$		Buxton et al. (1986)
H266③	$HOI + HSO_3^- \rightarrow H^+ + I^- + HSO_4^-$	$5.00 \cdot 10^9$		Pechtl and von Glasow (2007)
H267	$HOI + OH \rightarrow IO + H_2O$	$7.00 \cdot 10^9$		Buxton and Mulazzani (2007)
H268③	$INO_3 \rightarrow HOI + HNO_3$	$1.62 \cdot 10^6$	2800	Hoffmann et al. (2019b)
H269	$I_2O_2 + H^+ \rightarrow HIO_3 + HOI + H^+$	$3.20 \cdot 10^4$		Valkai and Horvath (2016)
H270	$IO_3^- + OH \rightarrow IO + O_2 + OH^-$	$1.08 \cdot 10^5$		Mezyk (1996)

(a) k_{298}^{2nd} in $l^1\ mol^{-1}\ s^{-1}$; k_{298}^{1st} in s^{-1}; (b) in K

Table S10 Implemented aqueous-phase equilibrium reactions in the CAPRAM-HM3.0red

② reactions that run in the cloud mode 'sub#1', ③ reactions that run in the aerosol mode 'sub#2', ● already included in CAPRAM3.0red

	Reaction	K[(a)]	$k_{f,\,298}$[(b)]	E_A/R[(c)]	$k_{b,\,298}$[(b)]	E_A/R[(c)]	References
H271②●	$Cl + Cl^- \rightleftharpoons Cl_2^-$	$1.4\cdot10^{5}$	$8.50\cdot10^{9}$		$6.00\cdot10^{4}$		Buxton et al. (1998)
H272③●	$Cl_2 + H_2O \rightleftharpoons H^+ + Cl^- + HOCl$	$1.90\cdot10^{-5}e^{-4500/T}$	$4.00\cdot10^{-1}$	8000	$2.10\cdot10^{4}$	3500	Wang and Margerum (1994)
H273③●	$HCl \rightleftharpoons H^+ + Cl^-$	$1.72\cdot10^{6}\ e^{6890/T}$	$5.00\cdot10^{11}$	-6890	$2.90\cdot10^{5}$		Marsh and McElroy (1985); Graedel and Weschler (1981)
H274②●	$Cl^- + OH \rightleftharpoons ClOH^-$	$7.00\cdot10^{-1}$	$4.30\cdot10^{9}$		$6.10\cdot10^{9}$		Jayson et al. (1973)
H275②	$Cl + OH^- \rightleftharpoons ClOH^-$	$7.83\cdot10^{8}$	$1.80\cdot10^{10}$		$2.30\cdot10^{1}$		Klaning and Wolff (1985)
H276②●	$ClOH^- + H^+ \rightleftharpoons Cl + H_2O$	$5.10\cdot10^{6}$	$2.1\cdot10^{10}$		$4.10\cdot10^{3}$		Jayson et al. (1973)
H277②●	$ClOH^- + Cl^- \rightleftharpoons Cl_2^- + OH^-$	$2.20\cdot10^{-4}$	$1.00\cdot10^{4}$		$4.50\cdot10^{7}$		Grigor'ev et al. (1987)
H278②●	$Cl^- + SO_4^- \rightleftharpoons Cl + SO_4^{2-}$	$1.20\cdot10^{0}$	$2.52\cdot10^{8}$		$2.10\cdot10^{8}$		Buxton et al. (1999b)
H279②●	$Cl^- + NO_3 \rightleftharpoons Cl + NO_3^-$	$3.40\cdot10^{0}\ e^{-4300/T}$	$3.40\cdot10^{8}$	4300	$1.00\cdot10^{8}$		Buxton et al. (1999a)
H280	$HOCl + NO_2^- \rightleftharpoons ClNO_2 + OH^-$	$3.97\cdot10^{-4}$	$1.99\cdot10^{7}$		$5.00\cdot10^{10}$		Lahoutifard et al. (2002)
H281③	$Cl_2 + SO_4^{2-} \rightleftharpoons Cl^- + HOCl + HSO_4^-$	$1.14\cdot10^{-3}$	$3.20\cdot10^{1}$		$2.80\cdot10^{3}$		Wang and Margerum (1994)
H282③●	$Cl^- + NO_2^+ \rightleftharpoons ClNO_2$	$1.44\cdot10^{8}$	$3.90\cdot10^{10}$		$2.70\cdot10^{2}$		Behnke et al. (1997)
H283②●	$Br + Br^- \rightleftharpoons Br_2^-$	$6.32\cdot10^{5}$	$1.20\cdot10^{10}$		$1.90\cdot10^{4}$		Merenyi and Lind (1994)
H284③	$Br_2 + H_2O \rightleftharpoons H^+ + Br^- + HOBr$	$1.06\cdot10^{-10}e^{-7500/T}$	$1.70\cdot10^{0}$	7500	$1.60\cdot10^{10}$		Beckwith et al. (1996)
H285③	$HBr \rightleftharpoons H^+ + Br^-$	$1.00\cdot10^{9}$	$5.00\cdot10^{11}$		$5.00\cdot10^{2}$		Lax (1969)
H286②●	$Br^- + OH \rightleftharpoons BrOH^-$	$3.33\cdot10^{2}$	$1.10\cdot10^{10}$		$3.30\cdot10^{7}$		Zehavi and Rabani (1972)
H287②	$Br + OH^- \rightleftharpoons BrOH^-$	$3.10\cdot10^{3}$	$1.30\cdot10^{10}$		$4.20\cdot10^{6}$		Zehavi and Rabani (1972); Klaning and Wolff (1985)
H288②●	$BrOH^- + H^+ \rightleftharpoons Br + H_2O$	$1.80\cdot10^{12}$	$4.40\cdot10^{10}$		$2.45\cdot10^{-2}$		Zehavi and Rabani (1972); Klaning and Wolff (1985)
H289②●	$BrOH^- + Br^- \rightleftharpoons Br_2^- + OH^-$	$7.00\cdot10^{1}$	$1.90\cdot10^{8}$		$2.70\cdot10^{6}$		Zehavi and Rabani (1972); de Violet (1981)
H290	$HOBr + HOBr \rightleftharpoons H^+ + Br^- + BrO_2^-$	$6.70\cdot10^{-12}$	$2.00\cdot10^{-5}$		$3.00\cdot10^{6}$		Field and Foersterling (1986)
H291	$HOBr + BrO_2^- \rightleftharpoons H^+ + Br^- + BrO_3^-$	$1.70\cdot10^{0}$	$3.20\cdot10^{0}$		$2.00\cdot10^{0}$		Field and Foersterling (1986)
H292②	$CH_2BrCOOH \rightleftharpoons CH_2BrCOO^- + H^+$	$1.75\cdot10^{-5}\ e^{46/T}$	$8.75\cdot10^{5}$	-46	$5.00\cdot10^{10}$		Bräuer et al. (2013)
H293③	$Br_2 + SO_4^{2-} + H_2O \rightleftharpoons HOBr + Br^- + HSO_4^-$	$6.15\cdot10^{-6}$	$2.28\cdot10^{4}$		$3.70\cdot10^{9}$		Beckwith et al. (1996)
H294③	$BrCl \rightleftharpoons HOBr + H^+ + Cl^- - H_2O$	$1.80\cdot10^{-5}$	$1.00\cdot10^{5}$		$5.60\cdot10^{9}$		Wang et al. (1994)
H295③	$BrCl^- \rightleftharpoons Br^- + Cl$	$1.60\cdot10^{-7}$	$1.90\cdot10^{3}$		$1.20\cdot10^{10}$		Donati (2002)

② reactions that run in the cloud mode 'sub#1', ③ reactions that run in the aerosol mode 'sub#2', ● already included in CAPRAM3.0red							
	Reaction	**K(a)**	**$k_{f,\,298}$(b)**	**E_A/R(c)**	**$k_{b,\,298}$(b)**	**E_A/R(c)**	**References**
H296③	$BrCl^- \rightleftharpoons Br + Cl^-$	$6.10\cdot10^{-4}$	$6.10\cdot10^{4}$		$1.00\cdot10^{8}$		Donati (2002)
H297③	$BrCl^- + Br^- \rightleftharpoons Br_2^- + Cl^-$	$1.86\cdot10^{3}$	$8.00\cdot10^{9}$		$4.30\cdot10^{6}$		Ershov (2004)
H298③	$BrCl^- + Cl^- \rightleftharpoons Br^- + Cl_2^-$	$2.75\cdot10^{-8}$	$1.10\cdot10^{2}$		$4.00\cdot10^{9}$		Ershov (2004)
H299③	$Br_2Cl^- \rightleftharpoons BrCl + Br^-$	$5.60\cdot10^{-5}$	$4.30\cdot10^{5}$		$7.70\cdot10^{9}$		Wang et al. (1994)
H300③	$Br_2Cl^- \rightleftharpoons Br_2 + Cl^-$	$7.60\cdot10^{-1}$	$3.80\cdot10^{4}$		$5.00\cdot10^{4}$		Wang et al. (1994); Matthew and Anastasio (2006)
H301③	$BrCl_2^- \rightleftharpoons BrCl + Cl^-$	$1.70\cdot10^{-1}$	$1.70\cdot10^{5}$		$1.00\cdot10^{6}$		Ershov (2004)
H302③	$BrCl_2^- \rightleftharpoons Br^- + Cl_2$	$1.50\cdot10^{-6}$	$9.00\cdot10^{3}$		$6.00\cdot10^{9}$		Ershov (2004)
H303	$I_2 + OH^- \rightleftharpoons I_2OH^-$	$5.00\cdot10^{0}$	$1.00\cdot10^{10}$		$2.00\cdot10^{9}$		Buxton and Mulazzani (2007)
H304	$I_2OH^- \rightleftharpoons HOI + I^-$	$8.30\cdot10^{0}$	$2.49\cdot10^{9}$		$3.00\cdot10^{8}$		Buxton and Mulazzani (2007)
H305	$HOI + H^+ + I^- \rightleftharpoons I_2 + H_2O$	$1.47\cdot10^{12}$	$4.40\cdot10^{12}$		$3.00\cdot10^{0}$		Eigen and Kustin (1962)
H306②	$HIO_3 \rightleftharpoons H^+ + IO_3^-$	$1.70\cdot10^{-1}$	$8.50\cdot10^{9}$		$5.00\cdot10^{10}$		Lide et al. (1995)
H307③	$HOI + H^+ + Cl^- \rightleftharpoons ICl$	$1.20\cdot10^{4}$	$2.90\cdot10^{10}$		$2.40\cdot10^{6}$		Wang et al. (1989)
H308③	$HOI + H^+ + Br^- \rightleftharpoons IBr$	$5.10\cdot10^{6}$	$4.10\cdot10^{12}$		$8.00\cdot10^{5}$		De Barros Faria et al. (1993)
H309③	$ICl + Br^- \rightleftharpoons IBr + Cl^-$	$3.30\cdot10^{3}$	$1.65\cdot10^{14}$		$5.00\cdot10^{10}$		Wagman et al. (1982)

(a) in M^{m-n}, n order of reaction of forward reaction, m order of reaction of backward reaction; (b) k_{298}^{2nd} in l^1 mol^{-1} s^{-1}, k_{298}^{1st} in s^{-1}; (c) in K

Table S11 Measured values of HCl and BrO in marine environments.

HCl	BrO*	Location	Comment	Reference
daily average: 133 – 675 ppt		Bermuda		Keene and Savoie (1999)
range: 30-250 ppt		Hawaii		Pszenny et al. (2004)
median: 351 ppt		Appledore Island		Keene et al. (2007)
daily median: 82-682 ppt		North to South Atlantic		Keene et al. (2009)
median: 206 ppt		Cape Verde	range: 26 – 613 ppt	Sander et al. (2013)
	max. 1-3.6 ppt	Canary Island	in remote ocean below detection limit	Leser et al. (2003)
	average 2.3 ppt	Mace Head	Coastal region	Saiz-Lopez et al. (2004)
	average max. 2.5 ± 1.1 ppt	Cape Verde		Read et al. (2008)
	< 0.5 ppt	Eastern tropical Pacific	MBL: below detection limit	Volkamer et al. (2015)
	0.03 ± 0.26 ppt	Western tropical Pacific	clean MBL outflow	Chen et al. (2016)
	0.17-1.64 ppt	Western Pacific	between 0.5 – 7 km height	Le Breton et al. (2017)

DL – Detection Limit; * for a more detailed overview on measurements before 2003 see Sander et al. (2003)

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