Supplement of Sensitivity of tropospheric ozone in LMDz-INCA vNMHC to halogenated chemistry

Table S1. List of halogen tracers in INCA.

#	**Tracer**	**description**	**ch.**[a]	**a/c**[b]	**em.**[c]	**d.d.**[d]	**w.s.**[e]
1	Br_2	Dibromine	●	●	-	●	●
2	Br	Bromine	●	-	-	-	-
3	BrO	Bromine monoxide	●	-	-	-	-
4	$HOBr$	Hypobromous acid	●	●	-	●	●
5	HBr	Hydrogen bromide	●	●	-	●	●
6	$BrNO_2$	Bromine nitrite	●	●	-	●	●
7	$BrNO_3$	Bromine nitrate	●	●	-	●	●
8	CH_3Br	Bromomethane	●	●	●	-	-
9	CH_2Br_2	Dibromomethane	●	●	●	-	-
10	I_2	Diiodine	●	●	●	●	●
11	I	Iodine	●	-	-	-	-
12	IO	Iodine monoxide	●	-	-	-	-
13	OIO	Dioxidoiodine	●	-	-	-	-
14	HOI	Hypoiodous acid	●	●	●	●	●
15	HI	Hydrogen iodide	●	●	-	●	●
16	INO	Nitrosyl iodide	●	●	-	-	-
17	INO_2	Iodine nitrite	●	●	-	●	●
18	INO_3	Iodine nitrate	●	●	-	●	●
19	CH_3I	Iodomethane	●	●	●	-	-
20	CH_2I_2	Diiodomethane	●	●	●	-	-
21	I_2O_2	Iodooxy hypoiodite	●	●	-	●	●
22	I_2O_3	Iodo iodate	●	●	-	●	●
23	I_2O_4	Iodosyl iodate	●	●	-	●	●
24	I_{aer}	Aerosol iodine	-	●	-	●	●
25	Cl_2	Dichlorine	●	●	-	●	●
26	Cl	Chlorine	●	-	-	-	-
27	HCl	Hydrogen chloride	●	●	●	●	●
28	ClO	Chlorine monoxide	●	-	-	-	-
29	$ClNO_2$	Chlorine nitrite	●	●	■	●	●
30	$ClNO_3$	Chlorine nitrate	●	●	-	●	●
31	$ClOO$	Chlorine superoxide	●	-	-	-	-
32	$OClO$	Chlorine dioxide	●	-	-	-	-
33	$HOCl$	Hydrochlorous acid	●	●	-	●	●
34	Cl_2O_2	Dichlorine dioxide	●	●	-	-	-
35	CH_3Cl	Chloromethane	●	●	●	-	-
36	CH_2Cl_2	Dichloromethane	●	●	●	-	-
37	$CHCl_3$	Trichloromethane	●	●	●	-	-
38	CH_2IBr	Bromoiodomethane	●	●	●	●	-
39	CH_2ICl	Chloroiodomethane	●	●	●	●	-
40	IBr	Iodine monobromide	●	●	■	●	●
41	ICl	Iodine monochloride	●	●	■	●	●
42	$BrCl$	Bromine monochloride	●	●	-	●	●

[a] Species is subject to chemistry

[b] Species is subject to advection/convection

[c] Species has a surface source ● or a chemical source ■

[d] Species is subject to dry deposition

[e] Species is subject to wet deposition

Table S2. Photolysis reactions of halogens included in the scheme. * J_{29} $\varphi_2(\lambda < 308 \text{ nm}) = 0.6$, φ_2 (λ=308-364 nm) = $7.143 \times 10^{-3} \lambda \text{ (nm)} - 1.60$, $\varphi_2(\lambda > 364 \text{ nm}) = 1.0$ and J_{30}, $\varphi_{30}(\lambda) = 1 - \varphi_{29}(\lambda)$.

Number	Reaction	Quantum yield φ	Reference of absorption cross-section
J1	$Br_2 + hv \rightarrow 2Br$	1	Sander et al. (2011)
J2	$BrNO_2 + hv \rightarrow Br + NO_2$	1	Sander et al. (2011)
J3	$BrONO_2 + hv \rightarrow BrO + NO_2$	0.15	Sander et al. (2011)
J4	$BrONO_2 + hv \rightarrow Br + NO_2$	0.85	Sander et al. (2011)
J5	$BrO + hv \rightarrow Br$	1	Sander et al. (2011)
J6	$CH_3Br + hv \rightarrow Br$	1	Sander et al. (2011)
J7	$CH_2Br_2 + hv \rightarrow 2Br$	1	Sander et al. (2011)
J8	$CHBr_3 + hv \rightarrow 3Br$	1	Sander et al. (2011)
J9	$HOBr + hv \rightarrow Br + OH$	1	Sander et al. (2011)
J10	$BrCl + hv \rightarrow Br + Cl$	1	Sander et al. (2011)
J11	$CH_2IBr + hv \rightarrow I + Br$	1	Sander et al. (2011)
J12	$IBr + hv \rightarrow I + Br$	1	Sander et al. (2011)
J13	$CH_2I_2 + hv \rightarrow 2I$	1	Sander et al. (2011)
J14	$CH_3I + hv \rightarrow I$	1	Sander et al. (2011)
J15	$HOI + hv \rightarrow I + OH$	1	Sander et al. (2011)
J16	$INO_3 + hv \rightarrow I + NO_3$	1	Sander et al. (2011)
J17	$I_2 + hv \rightarrow 2I$	1	Sander et al. (2011)
J18	$INO_2 + hv \rightarrow I + NO_2$	1	Sander et al. (2011)
J19	$INO + hv \rightarrow I + NO$	1	Sander et al. (2011)
J20	$IO + hv \rightarrow I$	0.91	Sander et al. (2011)
J21	$OIO + hv \rightarrow I + O_2$	1	Sander et al. (2011)
J22	$ICl + hv \rightarrow I + Cl$	1	Sander et al. (2011)
J23	$CH_2ICl + hv \rightarrow I + Cl$	1	Sander et al. (2011)
J24	$CH_2Cl_2 + hv \rightarrow 2Cl$	1	Sander et al. (2011)
J25	$CH_3Cl + hv \rightarrow Cl + CH_3O_2$	1	Sander et al. (2011)
J26	$Cl_2O_2 + hv \rightarrow Cl + ClOO$	1	Sander et al. (2011)
J27	$Cl_2 + hv \rightarrow 2Cl$	1	Sander et al. (2011)
J28	$ClNO_2 + hv \rightarrow Cl + NO_2$	1	Sander et al. (2011)
J29	$ClONO_2 + hv \rightarrow Cl + NO_2$	*	Sander et al. (2011)
J30	$ClONO_2 + hv \rightarrow ClO + NO_2$	*	Sander et al. (2011)
J31	$ClOO + hv \rightarrow CLO + O_2$	1	Sander et al. (2011)
J32	$ClO + hv \rightarrow Cl$	1	Sander et al. (2011)
J33	$HOCl + hv \rightarrow Cl + OH$	1	Sander et al. (2011)
J34	$OClO + hv \rightarrow ClO + O$	1	Sander et al. (2011)
J35	$I_2O_2 + hv \rightarrow I + OIO$	0.21	Gómez Martin et al. (2005); Spietz et al. (2005)
J36	$I_2O_3 + hv \rightarrow IO + OIO$	0.21	Gómez Martin et al. (2005); Spietz et al. (2005)
J37	$I_2O_4 + hv \rightarrow 2\ OIO$	0.21	Gómez Martin et al. (2005); Spietz et al. (2005)

Table S3. Bimolecular halogen reactions included in scheme. The scheme includes reations integrated in GEOS-Chem (Parrella et al., 2012; Eastham et al., 2014; Schmidt et al., 2016; Sherwen et al., 2016a; Sherwen et al., 2016b), TOMCAT (Hossaini et al., 2016) and Thomas et al., 2011. Species names are detailed in Folberth et al., 2006.

Nbr	Reaction	A$_0$ (molécules^{-2}cm^{6}s^{-1})	-E$_a$/R (K)	Reference
R1	$Cl + CH_3O_2 \rightarrow ClO + CH_2O + HO_2$	1.60 x 10^{-10}		Sander et al. (2011)
R2	$Cl + CH_3OOH \rightarrow HCl + CH_3O_2$	5.70 x 10^{-11}		Sander et al. (2011)
R3	$Cl + C_2H_6 \rightarrow HCl + C_2H_5O_2$	7.20 x 10^{-11}	-70	Sander et al. (2011)
R4	$Cl + C_2H_5O_2 \rightarrow ClO + HO_2 + CH_3CHO$	7.40 x 10^{-11}		Sander et al. (2011)
R5	$Cl + C_2H_5OH \rightarrow HCl + CH_3CHO$	9.60 x 10^{-11}		Sander et al. (2011)
R6	$Cl + CH_3COOH \rightarrow HCl + CH_3O_2 + CO_2$	2.80 x 10^{-14}		Sander et al. (2011)
R7	$Cl + C_3H_8 \rightarrow HCl + C_3H_7O_2$	7.85 x 10^{-11}	-80	Sander et al. (2011)
R8	$Cl + C_3H_8 \rightarrow HCl + PROPAO_2$	6.54 x 10^{-11}		Sander et al. (2011)
R9	$Cl + CH_3COCH_3 \rightarrow HCl + PROPAO_2$	7.70 x 10^{-11}		Sander et al. (2011)
R10	$Cl + ISOP \rightarrow HCl + ISOPO_2$	7.70 x 10^{-11}	500	Sander et al. (2011)
R11	$Cl + CH_3OH \rightarrow HCl + CH_2O + HO_2$	5.50 x 10^{-11}		Sander et al. (2011)
R12	$Cl + ALKAN \rightarrow HCl + ALKANO_2$	2.05 x 10^{-10}		Atkinson et al. (2006)
R13	$Cl + C_3H_6 \rightarrow HCl + PROPEO_2$	3.60 x 10^{-12}		Atkinson et al. (2006)
R14	$Cl + CH_3Cl \rightarrow CO + 2\ HCl + HO_2$	2.17 x 10^{-11}	-1130	Sander et al. (2011)
R15	$Cl + H_2O_2 \rightarrow HCl + HO_2$	1.10 x 10^{-11}	-980	Sander et al. (2011)
R16	$Cl + HO_2 \rightarrow HCl + O_2$	1.40 x 10^{-11}	270	Sander et al. (2011)
R17	$Cl + HO_2 \rightarrow ClO + OH$	3.60 x 10^{-11}	-375	Sander et al. (2011)
R18	$Cl + O_3 \rightarrow ClO + O_2$	2.30 x 10^{-11}	-200	Sander et al. (2011)
R19	$Cl + ClNO_3 \rightarrow Cl_2 + NO_3$	6.50 x 10^{-12}	135	Sander et al. (2011)
R20	$ClO + ClO \rightarrow Cl_2 + O_2$	1.00 x 10^{-12}	-1590	Sander et al. (2011)
R21	$ClO + ClO \rightarrow OClO + Cl$	3.50 x 10^{-13}	-1370	Sander et al. (2011)
R22	$ClO + ClO \rightarrow Cl + ClOO$	3.00 x 10^{-11}	-2450	Sander et al. (2011)
R23	$ClO + HO_2 \rightarrow O_2 + HOCl$	2.60 x 10^{-12}	290	Sander et al. (2011)
R24	$ClO + NO \rightarrow Cl + NO_2$	6.40 x 10^{-12}	290	Sander et al. (2011)
R25	$ClOO + Cl \rightarrow 2\ ClO$	1.20 x 10^{-11}		Sander et al. (2011)
R26	$ClOO + Cl \rightarrow Cl_2 + O_2$	2.30 x 10^{-10}		Sander et al. (2011)
R27	$ClO + CH_3O_2 \rightarrow ClOO + HO_2 + CH_2O$	3.30 x 10^{-12}	-115	Sander et al. (2011)
R28	$OH + CH_3Cl \rightarrow Cl + HO_2 + H_2O$	3.90 x 10^{-12}	-1411	Sander et al. (2011)
R29	$OH + CH_2Cl_2 \rightarrow 2\ Cl + HO_2 + H_2O$	1.90 x 10^{-12}	-870	Sander et al. (2011)
R30	$OH + CHCl_3 \rightarrow 3\ Cl + HO_2 + H_2O$	2.20 x 10^{-12}	-920	Sander et al. (2011)
R31	$OH + Cl_2 \rightarrow HOCl + Cl$	2.60 x 10^{-12}	-1100	Sander et al. (2011)
R32	$OH + Cl_2O_2 \rightarrow HOCl + ClOO$	6.00 x 10^{-13}	670	Sander et al. (2011)
R33	$OH + ClNO_2 \rightarrow HOCl + NO_2$	2.40 x 10^{-12}	-12 50	Sander et al. (2011)
R34	$OH + ClNO_3 \rightarrow HOCl + NO_3$	1.20 x 10^{-12}	-330	Sander et al. (2011)
R35	$OH + ClO \rightarrow HCl + O_2$	6.00 x 10^{-13}	230	Sander et al. (2011)
R36	$OH + ClO \rightarrow HO_2 + Cl$	7.40 x 10^{-12}	270	Sander et al. (2011)
R37	$OH + HCl \rightarrow H_2O + Cl$	1.80 x 10^{-12}	-250	Sander et al. (2011)
R38	$OH + HOCl \rightarrow H_2O + ClO$	3.00 x 10^{-12}	-500	Sander et al. (2011)
R39	$OH + OClO \rightarrow HOCl + O_2$	1.50 x 10^{-12}	600	Sander et al. (2011)
R40	$Cl + CH_4 \rightarrow HCl + CH_3O_2$	9.60 x 10^{-12}	-1360	Atkinson et al. (2004)

R41	$Cl + C_2H_4 \rightarrow HCl + C_2H_5O_2$	1.00×10^{-10}		Lurmann et al. (1986)
R42	$Cl + CH_2O \rightarrow HCl + HO_2 + CO$	8.10×10^{-11}	-30	Sander et al. (2003)
R43	$Cl + PAN \rightarrow HCl + CH_2O + NO_3$	1.00×10^{-14}		Sander et al. (2003)
R44	$Cl + HNO_3 \rightarrow HCl + NO_2$	1.00×10^{-16}		Sander et al. (2003)
R45	$Br + O_3 \rightarrow BrO + O_2$	1.60×10^{-11}	-780	Sander et al. (2011)
R46	$Br + HO_2 \rightarrow HBr + O_2$	4.80×10^{-12}	-310	Sander et al. (2011)
R47	$Br + CH_2O \rightarrow HO_2 + CO + HBr$	1.70×10^{-11}	-800	Sander et al. (2011)
R48	$Br + C_2H_6 \rightarrow C_2H_5O_2 + HBr$	2.36×10^{-10}	-6411	Seakins et al. (1992)
R49	$Br + C_3H_8 \rightarrow C_3H_7O_2 + HBr$	8.77×10^{-11}	-4330	Seakins et al. (1992)
R50	$Br + CH_3CHO \rightarrow CH_3CO_3 + HBr$	1.30×10^{-11}	-360	Atkinson et al. (2007)
R51	$Br + CH_3COCH_3 \rightarrow PROPAO_2 + HBr$	1.66×10^{-10}	-7000	King et al. (1970)
R52	$Br + C_3H_6 \rightarrow PROPEO_2 + HBr$	3.60×10^{-12}		Atkinson et al. (2006)
R53	$Br + ALKEN \rightarrow ALKENO_2 + HBr$	3.60×10^{-12}		Atkinson et al. (2006)
R54	$Br + BrNO_3 \rightarrow Br_2 + NO_3$	4.90×10^{-11}		Orlando and Tyndall (1996)
R55	$Br + NO_3 \rightarrow BrO + NO_2$	1.60×10^{-11}		Sander et al. (2011)
R56	$HBr + OH \rightarrow Br + H_2O$	5.50×10^{-12}	200	Sander et al. (2011)
R57	$BrO + OH \rightarrow Br + HO_2$	1.70×10^{-11}	250	Sander et al. (2011)
R58	$BrO + HO_2 \rightarrow HOBr + O_2$	4.50×10^{-12}	460	Sander et al. (2011)
R59	$BrO + NO \rightarrow Br + NO_2$	8.80×10^{-12}	260	Sander et al. (2011)
R60	$BrO + BrO \rightarrow 2 Br + O_2$	2.40×10^{-12}	40	Sander et al. (2011)
R61	$BrO + BrO \rightarrow Br_2 + O_2$	2.80×10^{-14}	860	Sander et al. (2011)
R62	$Br_2 + OH \rightarrow HOBr + Br$	2.10×10^{-11}	240	Sander et al. (2011)
R63	$CHBr_3 + OH \rightarrow 3 Br + CO$	1.35×10^{-12}	-600	Sander et al. (2011)
R64	$CH_2Br_2 + OH \rightarrow 2 Br + CO$	2.00×10^{-12}	-840	Sander et al. (2011)
R65	$CH_3Br + OH \rightarrow Br + CO$	2.35×10^{-12}	-1300	Sander et al. (2011)
R66	$I + O_3 \rightarrow IO + O_2$	2.10×10^{-10}	-830	Atkinson et al. (2007)
R67	$I + HO_2 \rightarrow HI + O_2$	1.50×10^{-11}	-1090	Sander et al. (2011)
R68	$I_2 + OH \rightarrow HOI + I$	2.10×10^{-10}		Atkinson et al. (2007)
R69	$HI + OH \rightarrow I + H_2O$	1.60×10^{-11}	440	Atkinson et al. (2007)
R70	$HOI + OH \rightarrow IO + H_2O$	5.00×10^{-12}		Riffault et al. (2005)
R71	$IO + HO_2 \rightarrow HOI + O_2$	1.40×10^{-11}	540	Atkinson et al. (2007)
R72	$IO + NO \rightarrow I + NO_2$	7.15×10^{-12}	300	Atkinson et al. (2007)
R73	$CH_3I + OH \rightarrow H_2O + I$	4.30×10^{-12}	-112 0	Atkinson et al. (2008)
R74	$INO + INO \rightarrow I_2 + 2 NO$	8.40×10^{-11}	-2620	Atkinson et al. (2007)
R75	$INO_2 + INO_2 \rightarrow I_2 + 2 NO_2$	4.70×10^{-12}	-1670	Atkinson et al. (2007)
R76	$I_2 + NO_3 \rightarrow I + INO_3$	1.50×10^{-12}		Atkinson et al. (2007)
R77	$INO_3 + I \rightarrow I_2 + NO_3$	9.10×10^{-11}	-146	Kaltsoyannis and Plane (2008
R78	$OIO + OIO \rightarrow I_2O_4$	1.50×10^{-10}		Gómez Martin et al. (2007)
R79	$OIO + NO \rightarrow NO_2 + IO$	1.10×10^{-12}	542	Atkinson et al. (2007)
R80	$IO + IO \rightarrow I + OIO$	2.16×10^{-11}	180	Atkinson et al. (2007)
R81	$IO + IO \rightarrow I_2O_2$	3.24×10^{-11}	180	Atkinson et al. (2007)
R82	$IO + OIO \rightarrow I_2O_3$	1.50×10^{-10}		Gómez Martin et al. (2007)

R83	I_2O_2 → IO + IO	1.00 x 10^{+12}	-9770	Ordóñez et al. (2012)
R84	I_2O_2 → OIO + I	2.50 x 10^{+14}	-9770	Ordóñez et al. (2012)
R85	I_2O_4 → 2 OIO	3.80 x 10^{-02}		Kaltsoyannis and Plane. (2008)
R86	INO_2 → I + NO_2	9.94 x 10^{+17}	-11859	McFiggans et al. (2000)
R87	INO_3 → IO + NO_2	2.10 x 10^{+15}	-13670	Kaltsoyannis and Plane. (2008)
R88	IO + ClO → I + OClO	2.59 x 10^{-11}	280	Atkinson et al. (2007)
R89	IO + ClO → I + Cl + O_2	1.18 x 10^{-12}	280	Atkinson et al. (2007)
R90	IO + ClO → ICl + O_2	9.40 x 10^{-13}	280	Atkinson et al. (2007)
R91	I + BrO → IO + Br	1.20 x 10^{-11}		Sander et al. (2011)
R92	IO + Br → I + BrO	2.70 x 10^{-11}		Bedjanian et al. (1997)
R93	IO + BrO → Br + I + O_2	3.00 x 10^{-12}	510	Atkinson et al. (2007)
R94	IO + BrO → Br + OIO	1.20 x 10^{-11}	510	Atkinson et al. (2007)
R95	ClO + BrO → OClO + Br	1.60 x 10^{-12}	430	Atkinson et al. (2004)
R96	ClO + BrO → Br + Cl + O_2	2.90 x 10^{-12}	220	Atkinson et al. (2004)
R97	ClO + BrO → BrCl + O_2	5.80 x 10^{-13}	170	Atkinson et al. (2004)
R98	IO + BrO → Br + I + O_2	3.00 x 10^{-12}	510	Atkinson et al. (2007)
R99	IO + BrO → Br + OIO	1.20 x 10^{-11}	510	Atkinson et al. (2007)

Table S4. Termolecular halogen reactions included in the scheme. This includes reactions from previous updates to halogen chemistry in GEOS-Chem (Parrella et al., 2012; Eastham et al., 2014; Schmidt et al., 2016; Sherwen et al., 2016a; Sherwen et al., 2016b). The lowerpressure limit rate (k0) is given by $A_0(\frac{300}{T})^x$. The high pressure limit is given by k∞. Fc characterises the fall off curve of the reaction as described by Atkinson et al. (2007).

Nbr	Termolecular reaction	A_0 (molecules^{-2}cm^{6}s^{-1})	x	k_∞	m	Fc	Reference
T1	$Cl + O_2 + M \rightarrow ClOO$	2.20×10^{-33}	0	1.80×10^{-10}	3.1	0.6	Sander et al. (2011)
T2	$ClO + ClO + M \rightarrow Cl_2O_2$	1.60×10^{-21}	2	3.0×10^{-12}	4.5	0.6	Sander et al. (2011)
T3	$ClO + NO_2 + M \rightarrow ClNO_3$	1.80×10^{-31}	3.4	1.50×10^{-11}	1.9	0.6	Sander et al. (2011)
T4	$ClOO + M \rightarrow Cl + O_2$	3.30×10^{-9}	0	2.73×10^{14}	3.1	0.6	Sander et al. (2011)
T5	$Cl_2O_2 + M \rightarrow Cl + O_2$	9.30×10^{-6}	2	1.74×10^{15}	4.5	0.6	Sander et al. (2011)
T6	$Cl + C_3H_6 + M \rightarrow ALKANO_2$	4.0×10^{-28}	0	2.80×10^{-10}	-	0.6	Atkinson et al. (2006)
T7	$Br + NO_2 + M \rightarrow BrNO_2$	4.20×10^{-31}	2.4	2.70×10^{-11}	-	0.6	Sander et al. (2011)
T8	$BrO + NO_2 + M \rightarrow BrNO_3$	5.20×10^{-31}	3.2	6.90×10^{-12}	-	0.6	Sander et al. (2011)
T9	$I + NO + M \rightarrow INO$	1.80×10^{-32}	1	1.70×10^{-11}	-	0.6	Atkinson et al.(2007)
T10	$I + NO_2 + M \rightarrow INO_2$	3.0×10^{-31}	1	6.60×10^{-11}	-	0.63	Atkinson et al.(2007)
T11	$IO + NO2 + M \rightarrow INO_3$	7.70×10^{-31}	5	1.60×10^{-11}	-	0.4	Atkinson et al.(2007)

Table S5. Halogen multiphase reactions and reactive uptake coefficients (γ).

Reaction	Reactive uptake coefficient on sea salt (γ)	Reactive uptake coefficient on sulfate aerosols (γ)
$HOBr + HBr \rightarrow Br_2 + H_2O$	0.2	0.2
$HOBr + HCl \rightarrow BrCl + H_2O$	0.2	0.2
$ClNO_3 + HBr \rightarrow BrCl + HNO_3$	0.2	0.2
$ClNO_3 \rightarrow HOCl + HNO_3$	0.001^a 0.01^b	0.001^a 0.01^b
$BrNO_3 \rightarrow HOBr + HNO_3$	0.03^a 0.8^b	0.03^a 0.8^b
$I_2O_x \rightarrow 2\ I_{aer}$	0.02	2.10^{-2}
$HI \rightarrow I_{aer}$	0.1	-
$HOI \rightarrow 0.85\ ICl + 0.15\ IBr + HNO_3$	0.01	-
$INO_3 \rightarrow 0.85\ ICl + 0.15\ IBr + HNO_3$	0.01	-
$INO_2 \rightarrow 0.85\ ICl + 0.15\ IBr + HNO_3$	0.02	-
$N_2O_5 \rightarrow 1.5\ HNO_3 + 0.5\ ClNO_2$	3.10^{-2}	-

[a] Uptake coefficient for moderate temperatures.

[b] Uptake coefficient for cold temperatures.

Table S6. Henry's law coefficients and molar heats of formation of halogen species.

Espèce	Henry's law contant (H) at 298 K in M/atm	Reference	d(lnH) / d(1/T) in K	Reference
HOBr	$1.9.10^{3}$	Frenzel et al., (1998)	$6.0.10^{3}$	McGrath and Rowland (1994)
HBr	$7.1.10^{13}$	Frenzel et al., (1998)	$1.02.10^{4}$	Schweitzer et al. (2000)
$BrNO_2$	0.3	Frenzel et al., (1998)	-	-
$BrNO_3$	10^{20}	Sander (2015)	-	-
Br_2	0.76	Dean (1992)	$3.72.10^{3}$	Dean (1992)
HOCl	$6.5.10^{3}$	Sander (2015)	$5.9.10^{3}$	Sander (2015)
HCl	$7.1.10^{15}$	Sander (2015)	$5.9.10^{3}$	Sander (2015)
$ClNO_3$	$2.69.10^{15}$	Sander (2015)	-	-
BrCl	0.97	Sander (2015)	-	-
ICl	$1.11.10^{2}$	Sander (2015)	$2.11.10^{3}$	Sander et al. (2006)
IBr	2.43.10	Sander (2015)	$4.92.10^{3}$	Sander et al. (2006)
HOI	$1.53.10^{3}$	Sander (2015)	$8.37.10^{3}$	Sander et al. (2006)
HI	$7.43.10^{13}$	Sander (2015)	$3.19.10^{3}$	Sander et al. (2006)
INO_3	$2.69.10^{15}$	Vogt et al. (1999)	$3.98.10^{4}$	Kaltsoyannis and Plane (2008)
I_2O_2	$2.69.10^{15}$	Analogie avec INO3	$1.89.10^{4}$	Kaltsoyannis and Plane (2008)
I_2	2.63	Sander (2015)	$7.51.10^{3}$	Sander et al. (2006)
INO_2	0.3	Analogie avec BrNO3	$7.24.10^{3}$	Sander et al. (2006)
I_2O_3	$2.69.10^{15}$	Analogie avec INO3	$7.7.10^{3}$	Kaltsoyannis and Plane (2008)
I_2O_4	$2.69.10^{15}$	Analogie avec INO3	$1.34.10^{4}$	Kaltsoyannis and Plane (2008)
Cl_2	0.086		2.10^{3}	Kavanaugh and Trussell (1980)
$ClNO_2$	0.024	Sander (2015)	-	Behnke et al. (1997)

Table S7. Primary emissions of organic chlorine (Gg Cl.an^{-1}) in LMDz-INCA and CAM-Chem.

Espèces	Plants between the extratropics (Gg Cl.an^{-1})	Biomass burning (Gg Cl.an^{-1})	Marine organic (Gg Cl.an^{-1})	Industrial (Gg Cl.an^{-1})	LMDz-INCA (Gg Cl.an^{-1})	CAM-Chem (Gg Cl.an^{-1})
CH_3Cl	1430	142	510	85	2166$^{b, e}$	2300^{a}
CH_2Cl_2	-	75	124	430	629$^{b, c}$	480^{a}
$CHCl_3$	-	-	236	79	315$^{b, d}$	260^{a}

a. Ordonez et al., 2012 ; Saiz-Lopez et al., 2012 ; Fernandez et al., 2014 ; Saiz Lopez et al., 2014

b. (WMO (World Meteorological Organization), Scientific Assessment of Ozone Depletion: 2014, World Meteorological Organization, Global Ozone Research and Monitoring Project-Report, 2014)

c. Xiao et al., 2007

d. Worton et al., 2006

e. Hu et al., 2013

Table S8. Chemical lifetime of primary halogenated compounds in LMDz-INCA and in the litterature.

Species	*Lifetime (+ hv / + OH) in LMDz-INCA*	*Lifetime in the litterature*
CH_3Br	1.7 years	1.6[b] / 1.5-1.8 years[c]
CH_2Br_2	137 days	100[d]/140[e] days
$CHBr_3$	25 days	20[d] / 15-37 days[e]
CH_3Cl	1.6 years	1.6 years[a]
CH_2Cl_2	157 days	144 days[a]
$CHCl_3$	163 days	149 days[a]
CH_2IBr	0.3 days	-
CH_2ICl	0.5 days	0.1 day[a]
CH_3I	5.9 days	Several days[f]
CH_2I_2	4.3 hours	3.6 hours[g]

a. Carpenter et al., 2014
b. Yvon-Lewis and Butler, 1997
c. Kinnison *et al.*, 2007
d. Kerkweg *et al.*, 2008
e. Liang *et al.*, 2009
f. V. Rattigan et al., 1997
g. C. Mössinger et al., 1998

Table S9. Comparison of reactive Chlorine Cl∗ (Cl_2, HOCl, $ClNO_2$, $ClNO_3$) between LMDz-INCA, GEOS-Chem and observations in oceanic regions. Measurements are 24h mean. Model outputs represent respective monthly means (2010 For LMDz-INCA and 2016 for GEOS-Chem) in the same location and date.

Location	**Months**	**Cl* simulated with GEOS-Chem (ppt)**	**Cl* simulated with LMDz-INCA (ppt)**	**Measured Cl* (ppt)**	**Reference**
Eastern Atlantic	Oct - Nov	43	80 (dont 72 $ClNO_2$)	27	Keene et al. (2009)
Atlantic near Northern Africa	Oct - Nov	5	14.2	<24	Keene et al. (2009)
Tropical Atlantic	Oct - Nov	2	1.4	<24	Keene et al. (2009)
Southern Atlantic	Oct - Nov	4	3.4	<24	Keene et al. (2009)
Appledore island	Juillet-Aout	17	1.4	<20	Keene et al. (2007)
Hawaii	Septembre	4	3.4	6	Pszenny et al. (2004)
Alert (Canada)	Mars - Avril	0.2	1.4	<14	Impey et al. (1999)

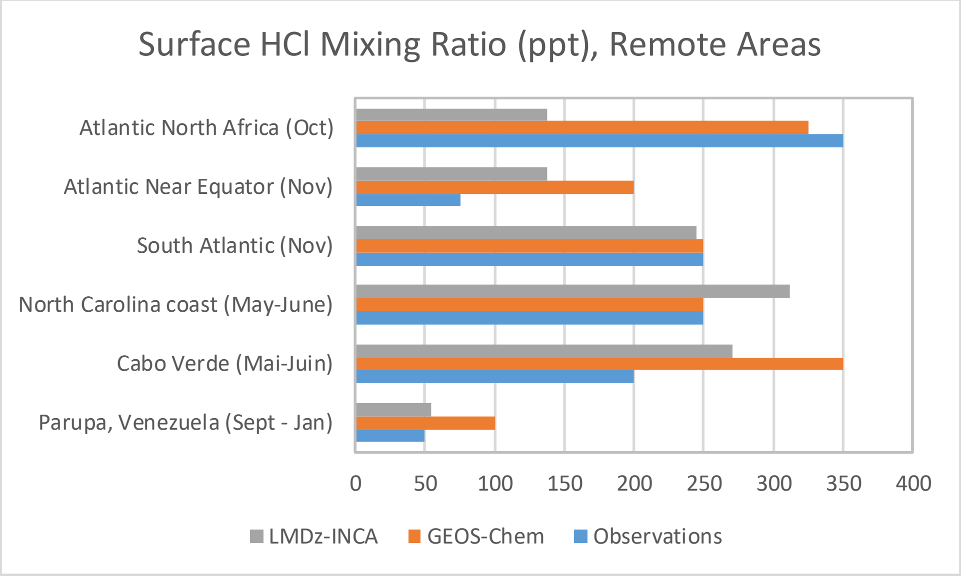

Figure S1. Average surface HCl mixing ratios from LMDz-INCA and GEOS-Chem (Wang et al., 2019) simulations as well as observations in coastal sites and oceanic areas.