Supplement of Geosci. Model Dev., 16, 4041–4062, 2023
https://doi.org/10.5194/gmd-16-4041-2023-supplement

Geoscientific Model Development
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Supplement of

Sensitivity of tropospheric ozone to halogen chemistry in the chemistry–climate model LMDZ-INCA vNMHC

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Table S1. Henry's law coefficients and molar heats of formation of halogen species.

Compound	Henry's law constant (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)

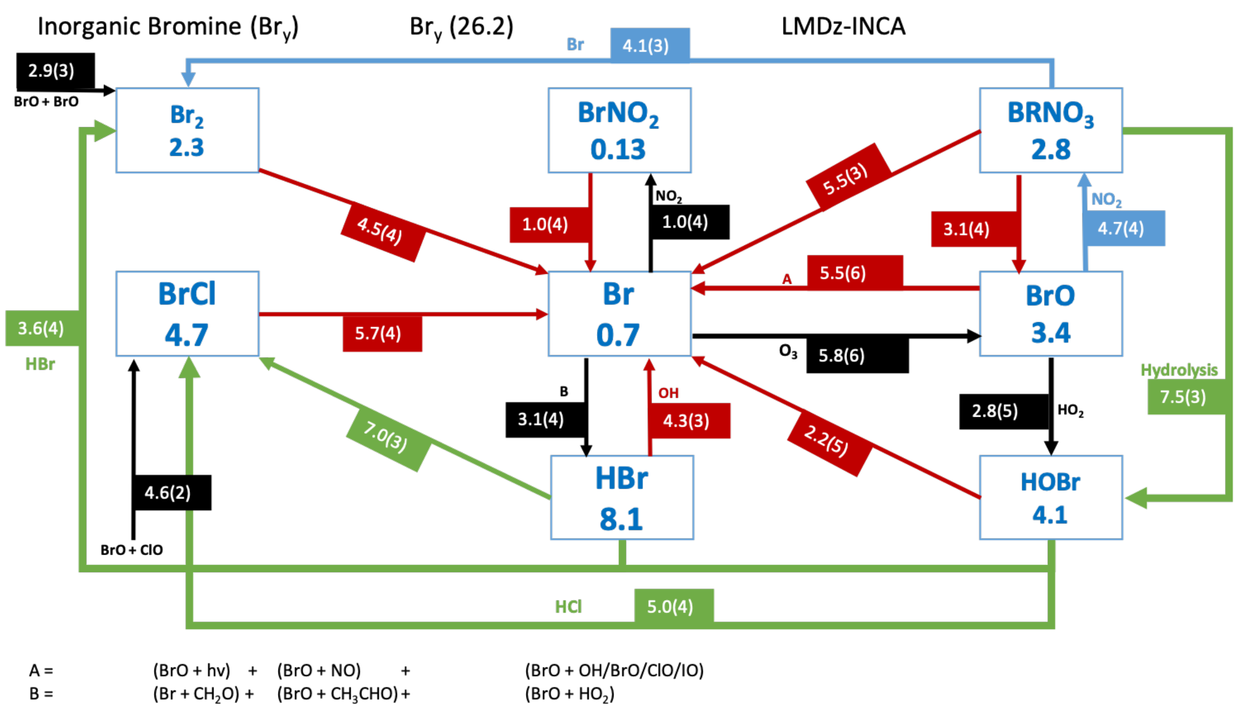
Table S2: Preindustrial and present-day surface emissions and methane concentrations considered in the LMDz-INCA simulations

Surface emissions (Tg/yr)	Preindustrial	Present
alkan	1,2	55,1
alken	1,8	9,0
isop	526,7	526,7
mek	1,1	3,3
mvk	0,0	1,4
apin	121,5	121,5
arom	12,7	45,4
C_2H_2	1,8	5,6
C_2H_4	6,1	13,3

C_2H_5OH	1,1	8,7
C_2H_6	3,7	8,7
C_3H_6	4,1	8,1
C_3H_8	0,9	6,3
CH_2O	9,2	13,9
CH_3CHO	19,0	22,1
CH_3COCH_3	60,7	62,9
CH_3OH	106,9	110,4
CO	432,4	971,7
NO	13,2	103,8
Tropospheric conenetations (in ppbv)		
CH_4	792	1800

Table S3. 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 means but each value represents a mean of several days of measurement. Model outputs represent respective monthly means (2010 for LMDZ-INCA and 2016 for GEOS-Chem) in the same location.

Location	Months	Cl* simulated with GEOS-Chem (ppt)	Cl* simulated with LMDz-INCA (ppt)	Measured Cl* (ppt)	Reference
Eastern Atlantic	Oct – Nov	43	80 (72 being $ClNO_2$)	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)



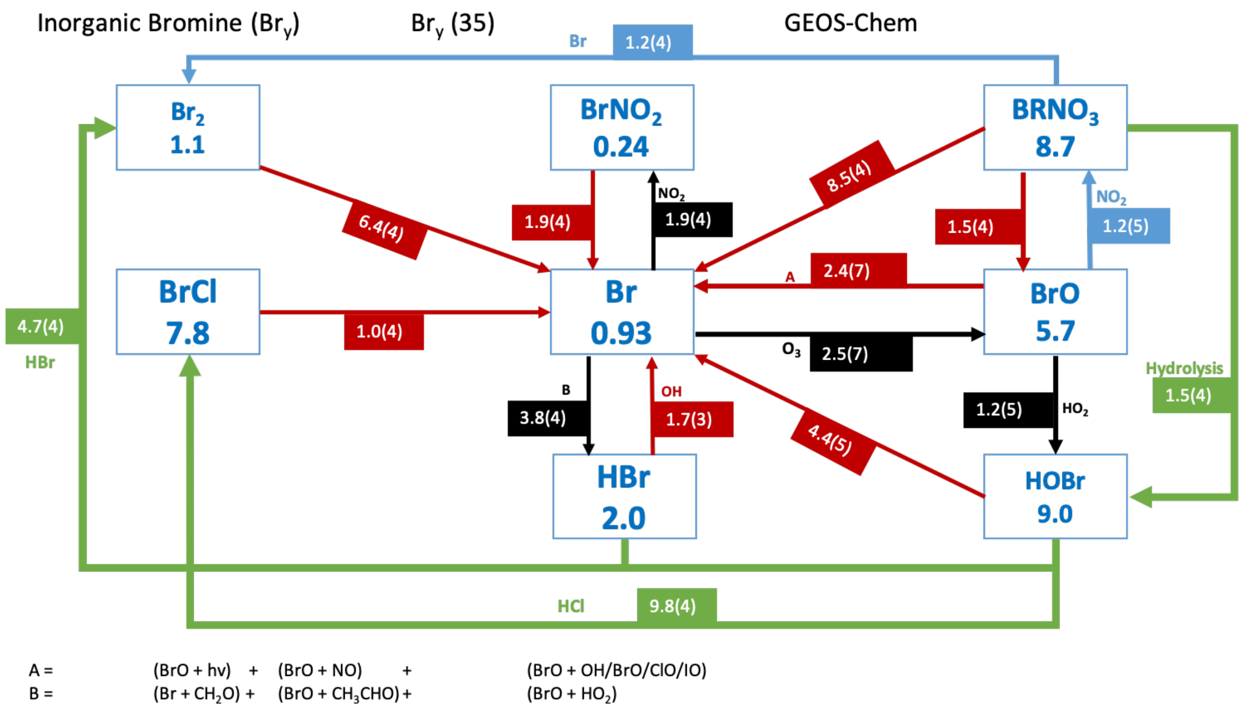


Figure S1 : Global budget and cycling of tropospheric bromine (Br_y) in LMDZ-INCA (this work, upper panel) and GEOS-Chem (from Schmidt et al. 2016, lower panel). Tropospheric global burden of inorganic bromines (Gg Br) and fluxes through reactions (Gg Br.yr-1) are indicated. Read 1.2 (4) as 1.2×10^4.

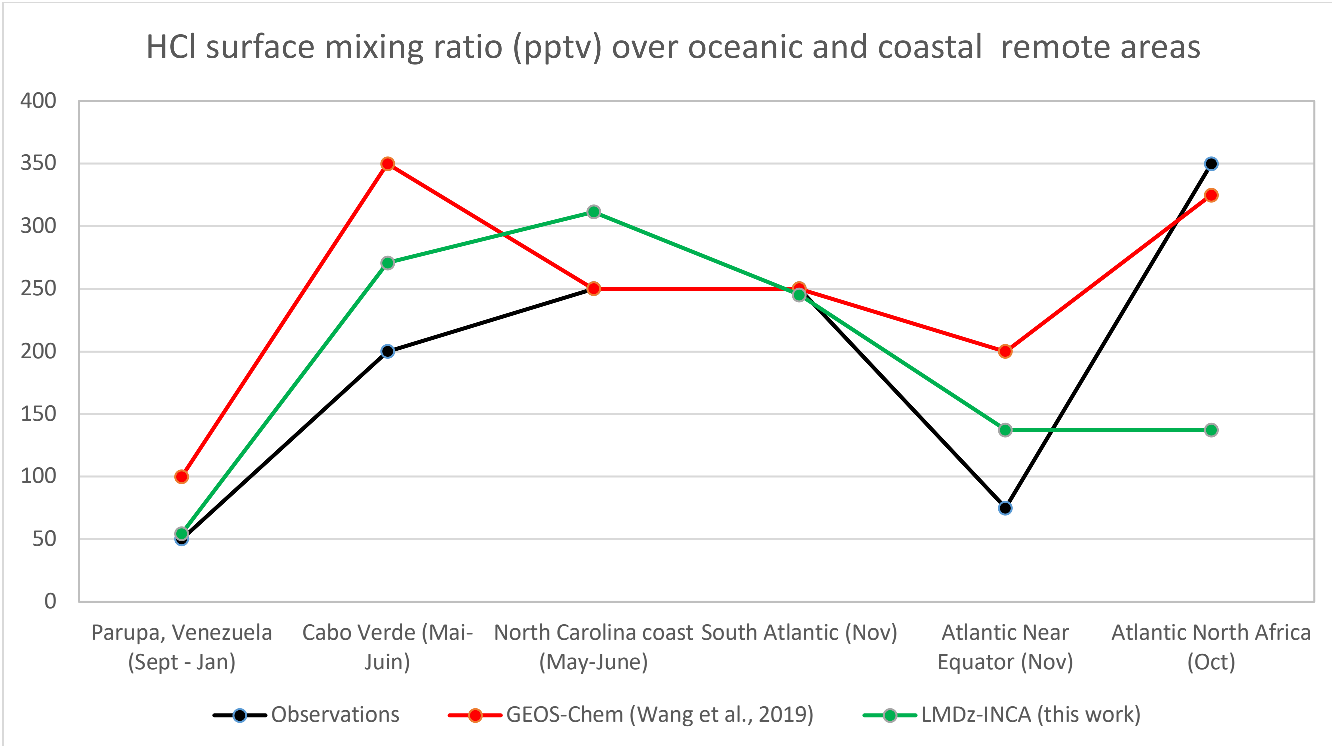


Figure S2. Average surface HCl mixing ratios from LMDz-INCA and GEOS-Chem (Wang et al., 2019) simulations as well as observations in coastal sites and oceanic areas. Observations are from Keene et al. (2009); Sanhueza and Garaboto (2002); Crisp et al. (2014) as reported by Wang et al. (2019).

Additional References for the Supplementary Material:

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