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Observation and modelling of ozone-destructive halogen chemistry in a passively degassing volcanic plume

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1 Figures

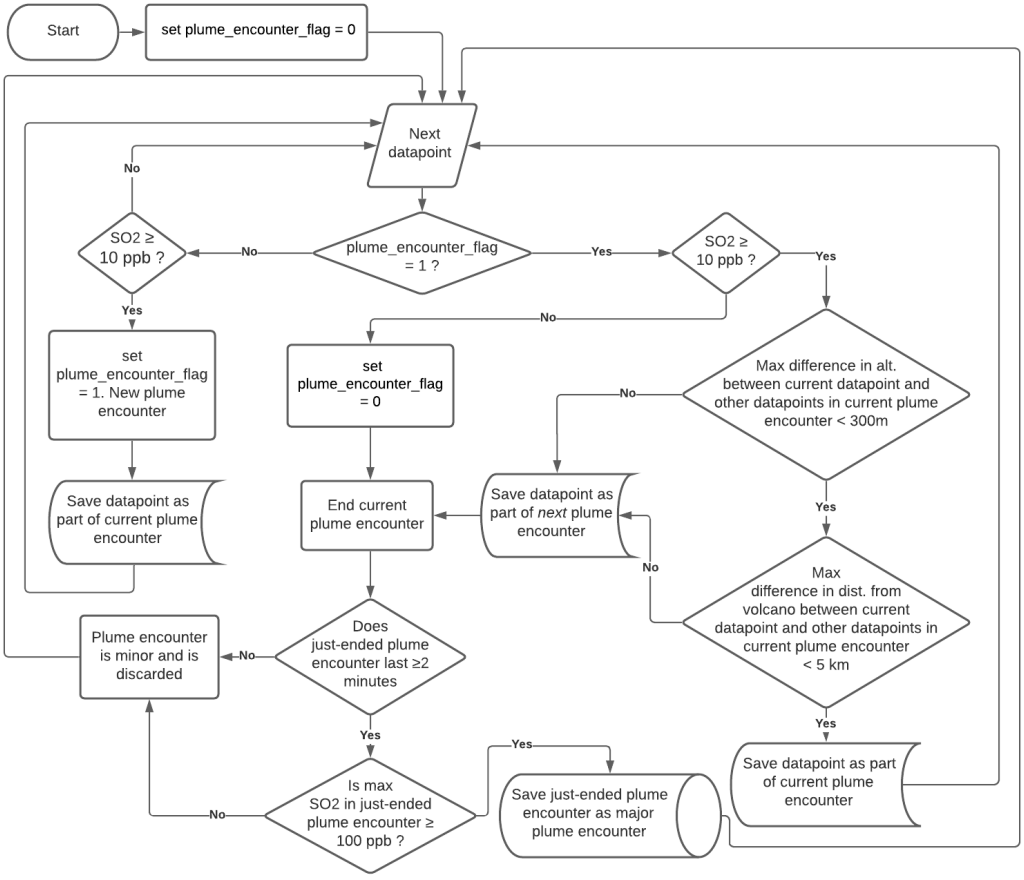

Figure S1. Flow chart representation of algorithm used to identify major plume encounters within the observational data.

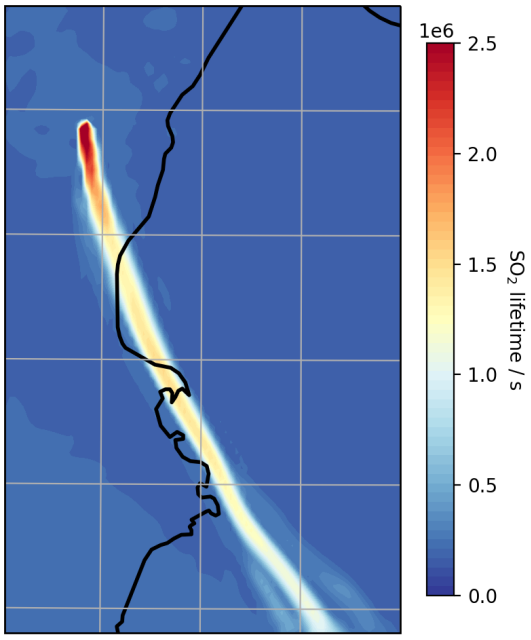

Figure S2. Modelled instantaneous lifetime of SO_2 at 3300mASL 0800 UTC on 2012-08-01.

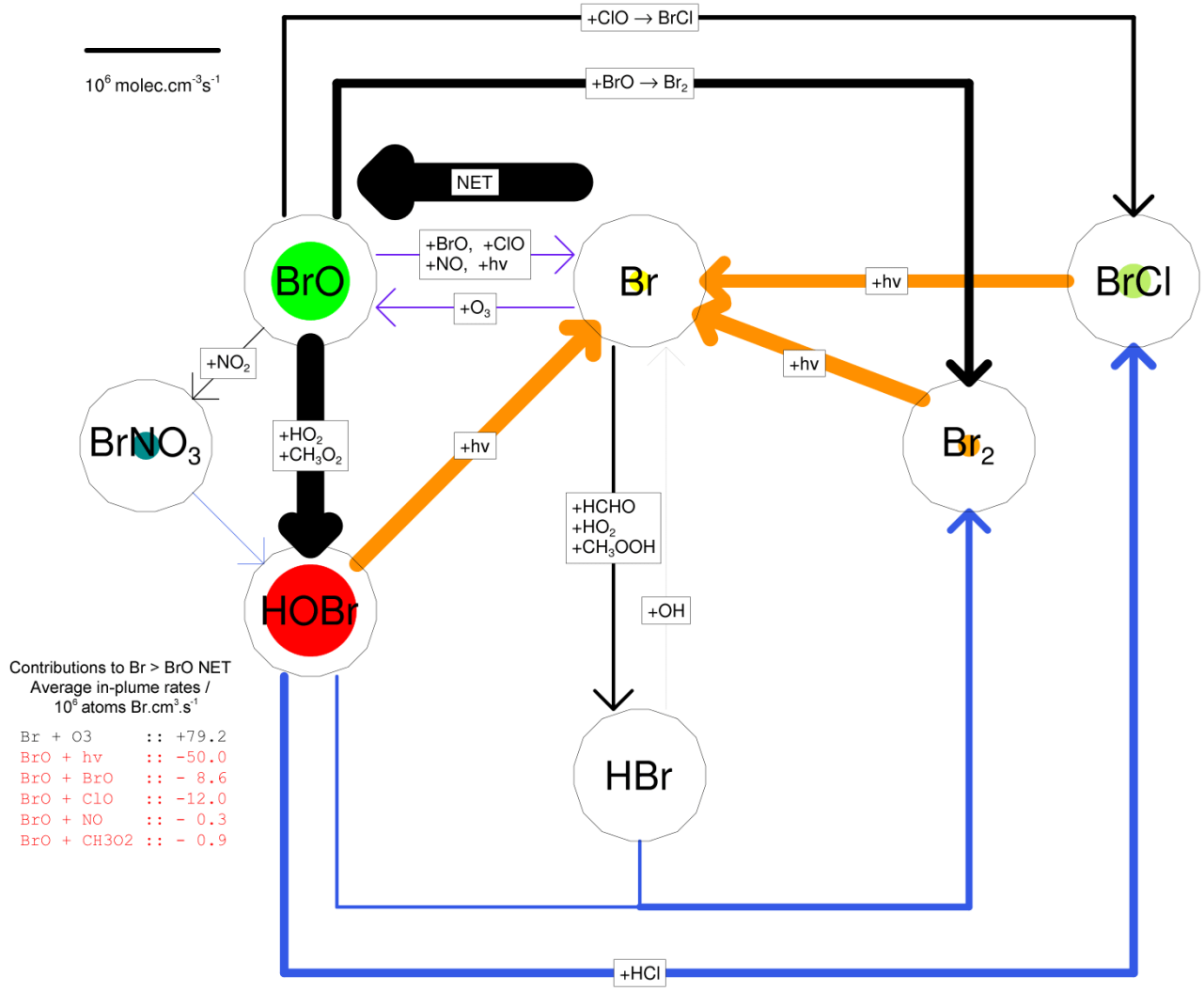

Figure S3. The in-plume bromine cycle in the plume for plume aged 30-60 minutes at 2012-08-01 0800. Areas of the coloured circles are proportional to the fraction of total bromine present as that species, a fully coloured circle would correspond to 100%. Widths of lines are proportional to the weighted average rate of these reactions in the plume, see reference line top left for scale. Orange lines indicate photolysis reactions, blue lines heterogeneous reactions, black lines other gas-phase reactions. The rates of reactions contributing to the Br $\rightleftharpoons$ BrO interchange are depicted bottom left, only the net Br $\longrightarrow$ BrO flux is shown.

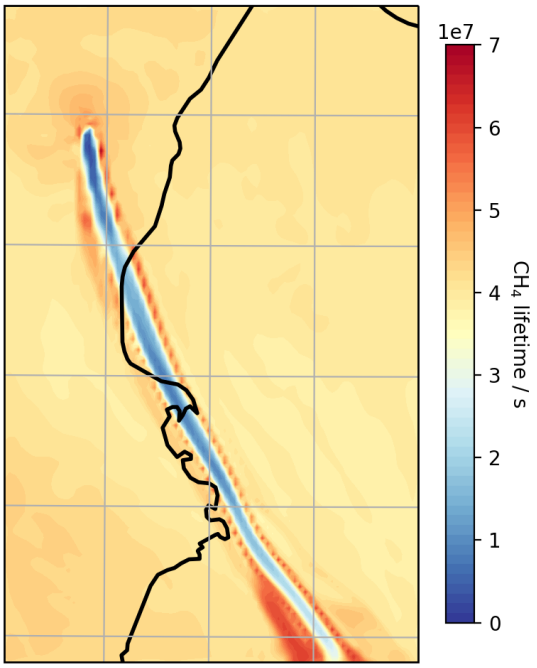

Figure S4. Modelled instantaneous lifetime of CH_4 at 3300mASL 0800 UTC on 2012-08-01.

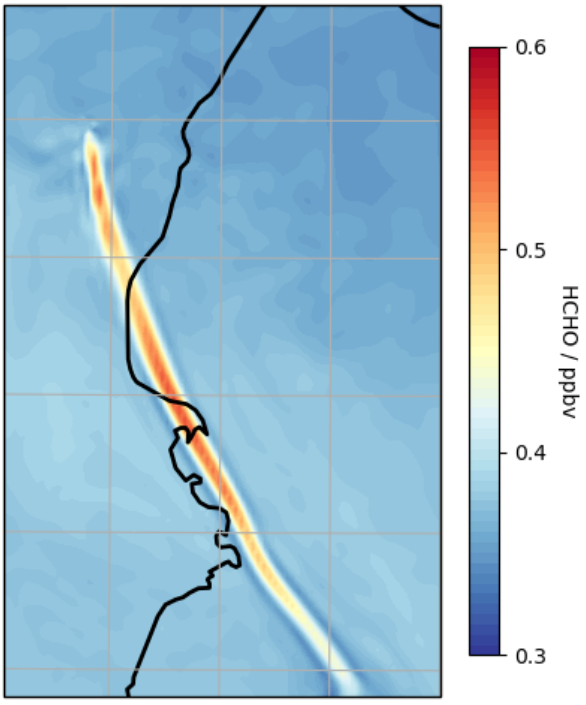

Figure S5. Modelled mixing ratio of HCHO at 3300mASL 0800 UTC on 2012-08-01.

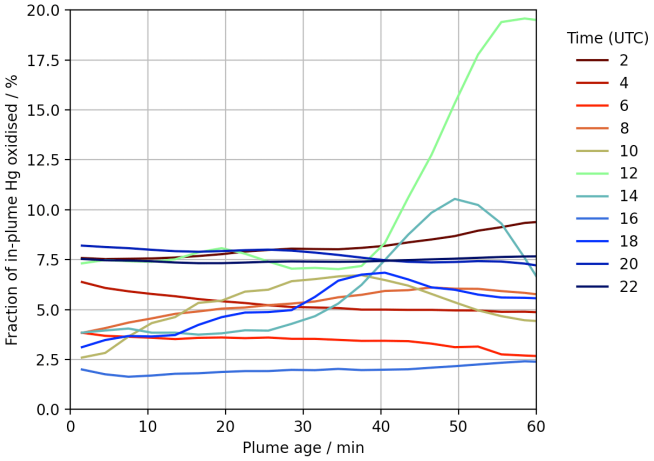

Figure S6. In-plume average percentage of Hg in oxidised forms for plume of different ages ranging from 0–60 minutes at several times on 2012-08-01. Note that these lines represent snapshots of the plume rather than Lagrangian traces

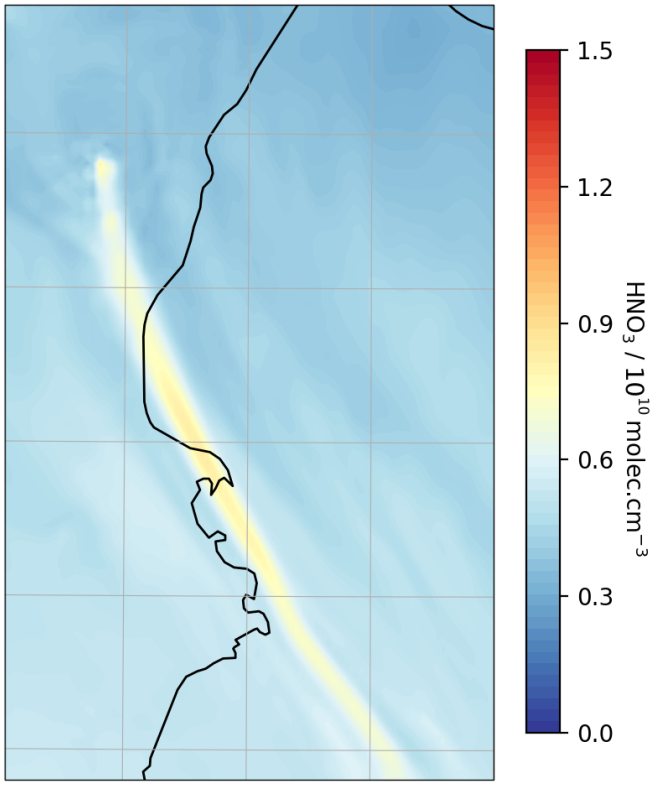

Figure S7. Model mixing ratio HNO3 at 3300mASL at 0800 UTC on 2012-08-01 from the *no_NO* model run

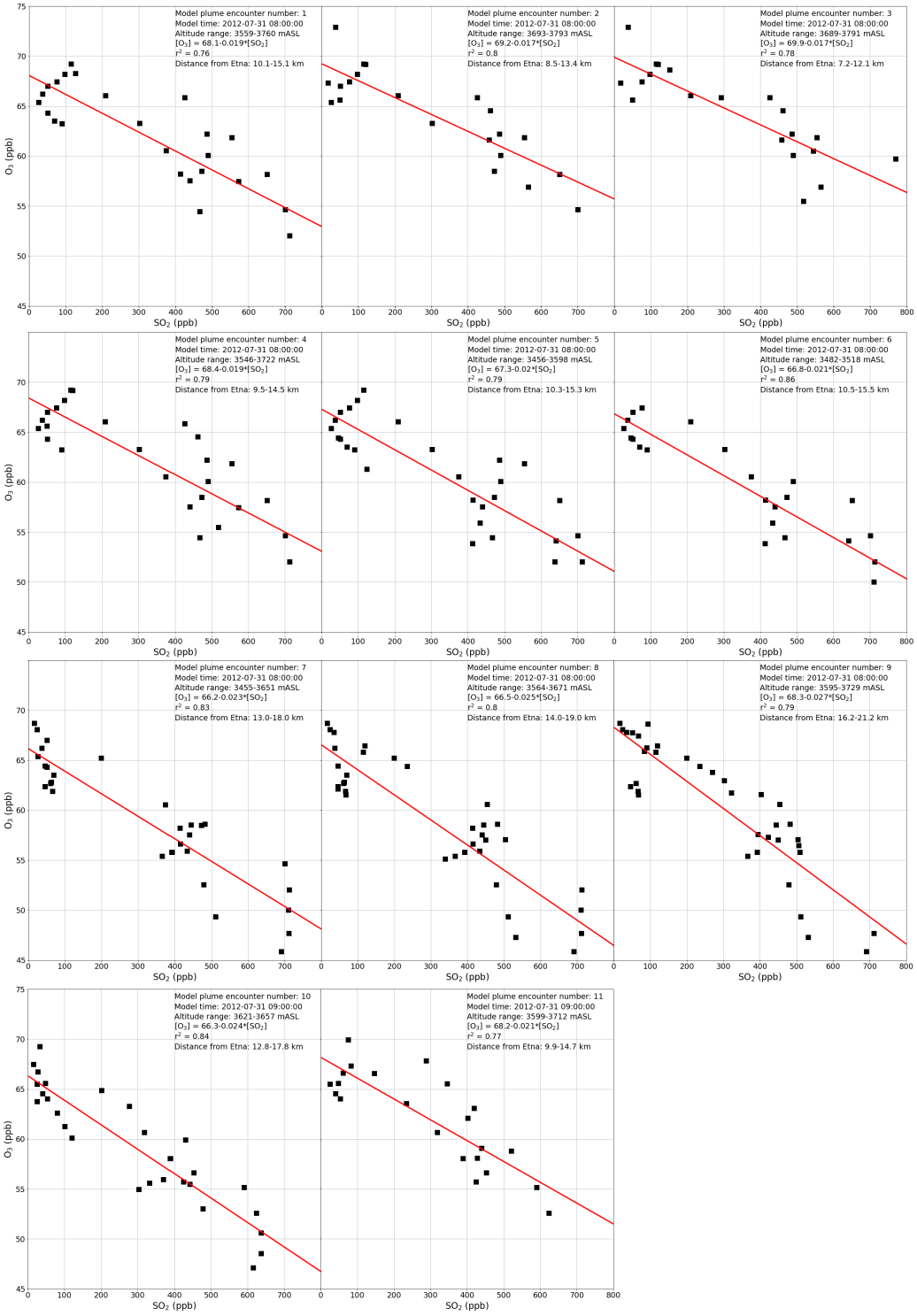

Figure S8. Modelled equivalent SO_2 and O_3 for the 11 major plume encounters on 2012-07-31.

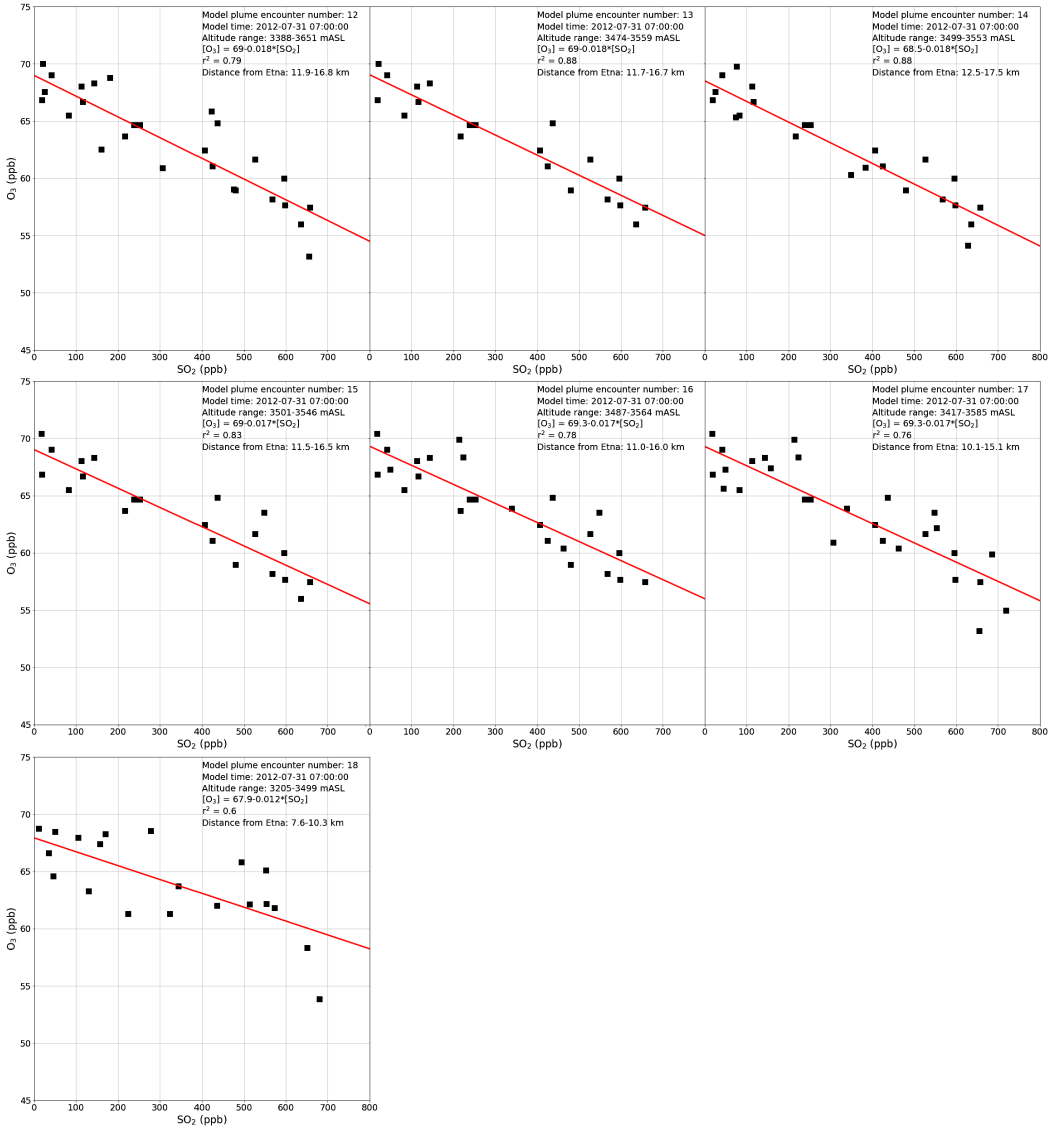

Figure S9. Modelled equivalent SO_2 and O_3 for the 8 major plume encounters on 2012-08-01.

2 Model chemical mechanism

The following tables list the reactions added to the CMBZ MOSAIC 8-bin mechanism to form the WCV mechanism. The main source for reaction rates are the values recommended by the IUPAC Task Group on Atmospheric Chemistry (http://iupac.pole-ether.fr: Atkinson et al., 2004, 2006, 2007, 2008; Crowley et al., 2010; Ammann et al., 2013), this source is referred to as "IUPAC" in the tables below.

Fractional quantities indicate reactions that account for multiple, branching reactions. O_2 is not included as a reaction product in the mechanism as it is not simulated by the model. Some short lived species, such as the H radical, are not expressly modelled; their products (e.g. $H + O_2 \rightarrow HO_2$) are considered to be formed directly by the mechanism. As such, some reactions do not balance stoichiometrically.

2.1 Photolysis

New photolysis reactions are tabulated in Table S1. hν indicates a photon.

Reactant		Products	Reference
BrO	$\xrightarrow{h\nu}$	Br + O_3	IUPAC
Br_2	$\xrightarrow{h\nu}$	2 Br	IUPAC
HOBr	$\xrightarrow{h\nu}$	Br + OH	IUPAC
$BrNO_2$	$\xrightarrow{h\nu}$	Br + NO_2	IUPAC
$BrNO_3$	$\xrightarrow{h\nu}$	Br + NO_3	IUPAC
OClO	$\xrightarrow{h\nu}$	ClO + O_3	IUPAC
Cl_2	$\xrightarrow{h\nu}$	2 Cl	IUPAC
HOCl	$\xrightarrow{h\nu}$	Cl + OH	IUPAC
$ClNO_2$	$\xrightarrow{h\nu}$	Cl + NO_2	IUPAC
$ClNO_3$	$\xrightarrow{h\nu}$	Cl + NO_3	IUPAC
BrCl	$\xrightarrow{h\nu}$	Br + Cl	IUPAC
HgBr	$\xrightarrow{h\nu}$	Hg + Br	Saiz-Lopez et al. (2019)
HgCl	$\xrightarrow{h\nu}$	Hg + Cl	Saiz-Lopez et al. (2019)
$HgBr_2$	$\xrightarrow{h\nu}$	HgBr + Br	Saiz-Lopez et al. (2018)
HgBrCl	$\xrightarrow{h\nu}$	HgCl + Br	*see below*

Table S1. Photolysis reactions of bromine and chlorine species in the WCV mechanism

To our knowledge no photolysis cross section has been published for HgBrCl. We assume photolysis rates of half that of $HgBr_2$ with Br radicals being produced as this is the weaker bond. Saiz-Lopez et al. (2018) report tropospheric lifetimes of $HgCl_2$ far in excess of the timescales of this study, we therefore exclude photolysis of this species.

2.2 Heterogeneous

WCV's reaction mechanism includes heterogeneous reactions (Table S2) where the reaction is assumed to take place between a gas-phase species and a species adsorbed onto or into the aerosol. We do not compute these by calculating the bulk aqueous-phase chemistry, but instead employ a reaction probability approach wherein the rate of a heterogeneous reaction is considered to be proportional to the rate of reactive uptake of the gas-phase species to the aerosol phase. We use the mechanism developed by Marelle et al. (2021) which also accounts for gas-phase diffusion effects and the approach of Jourdain et al. (2016) to determine the products of HOBr reactive uptake.

Reactant		Products
N_2O_5 + H_2O	$\longrightarrow$	2 HNO_3
$BrNO_3$ + H_2O	$\longrightarrow$	HOBr + HNO_3
$ClNO_3$ + H_2O	$\longrightarrow$	HOCl + HNO_3
HOBr + HBr	$\longrightarrow$	Br_2 + H_2O
HOBr + HCl	$\longrightarrow$	BrCl + H_2O

Table S2. Heterogeneous reactions in the WCV mechanism

The various coefficients used to calculate heterogeneous reaction rates are tabulated in Table S3. γ are uptake coefficients; the probability that the specified molecule, upon impacting an aerosol surface, undergoes a reaction. The D values below are values for the diffusivity of these species in air, which is used in calculations that account for local depletion of these species in the air around aerosol particles.

The concentration of HBr and HCl in particles is calculated on-line from the gas-phase concentrations of these species and their effective Henry's law coefficients (H′). Following HOBr uptake, the the branching ratio between the Br_2- and BrCl-producing pathways is calculated from these concentrations and the the equilibrium constants of the $BrCl + Br^- \overset{K_2}{\rightleftharpoons} Br_2Cl$ and $Br_2Cl^- \overset{K_3}{\rightleftharpoons} Br_2 + Cl$ reactions (Wang et al., 1994; Jourdain et al., 2016).

For HOBr, the recommended value for the accommodation coefficient (α), the fraction of gas-phase HOBr moculules taken onto or into the particles after collision, is 0.6 (Ammann et al., 2013). Experiments on sea-salt aerosol suggest that the uptake coefficient, is very close to the accommodation coefficient for acidic particles (Ammann et al., 2013). As volcanic aerosol is highly acidic, we set γ to be 0.6.

At standard temperatures, the value of $\frac{K_2}{K_3}\frac{H'_{HCl}}{H'_{HBr}}$ is about 10^{-7}, meaning that the branching will strongly favour Br_2 production unless HBr is nearly completely depleted within the plume.

Equivalent heterogeneous reactions for HOCl are not included in the model, as the uptake coefficient is reported to be <0.02 (Crowley et al., 2010).

Parameter	Value	Reference
γ_{HOBr}	0.6	IUPAC
$\gamma_{N_2O_5}$	0.03	IUPAC
γ_{BrNO_3}	0.8	Burkholder et al. (2015)
γ_{ClNO_3}	0.11	IUPAC
$D_{0,HOBr}$	11000 Pa cm^2 s^{-1}	Tang et al. (2014)
D_{0,N_2O_5}	8700 Pa cm^2 s^{-1}	
$D_{0,BrNO_3}$	36000 Pa cm^2 s^{-1}	Theoretical values calculated as per Tang et al. (2014)
$D_{0,ClNO_3}$	37000 Pa cm^2 s^{-1}	
H'_{HCl}	$2.0 \times 10^4 e^{9000(\frac{1}{T}-\frac{1}{298})}$ mol^2 m^{-6} Pa^{-1}	Brimblecombe and Clegg (1988, 1989), as reported by Sander (2015)
H'_{HBr}	$1.3 \times 10^7 e^{10000(\frac{1}{T}-\frac{1}{298})}$ mol^2 m^{-6} Pa^{-1}	
K_2	1.3 M^{-1}	Wang et al. (1994)
K_3	1.8×10^4 M^{-1}	

Table S3. Coefficients used to determine heterogeneous reaction rates and branching ratio of the HOBr reaction

2.3 Gas phase

Table S4 gives the other bromine, chlorine, and mercury reactions included in the WCV mechanism. T is temperature in K. [X] indicates the concentration of species X in molecules cm^{-3}. [M] indicates the total air concentration.

Table S4: Br, Cl, and Hg gas-phase reactions in the WCV mechanism.

Reactants		Products	Rate equation / s^{-1}	Reference
Br + O_3	$\longrightarrow$	BrO	$1.7 \times 10^{-11} e^{\frac{-800}{T}}$ [Br][O_3]	IUPAC
Br + HO_2	$\longrightarrow$	HBr	$7.7 \times 10^{-12} e^{\frac{-450}{T}}$ [Br][HO_2]	IUPAC
Br + HCHO	$\longrightarrow$	HBr + CO + HO_2	$7.7 \times 10^{-12} e^{\frac{-580}{T}}$ [Br][HCHO]	IUPAC
Br + CH_3OOH	$\longrightarrow$	CH_3O_2 + HBr	$2.7 \times 10^{-12} e^{\frac{-1610}{T}}$ [Br][HCHO]	von Glasow et al. (2004)
BrO + HO_2	$\longrightarrow$	HOBr	$4.5 \times 10^{-12} e^{\frac{500}{T}}$ [BrO][HO_2]	IUPAC
BrO + CH_3O_2	$\longrightarrow$	0.72 HOBR + 0.28 Br + 0.28 HO_2 + HCHO	$4.1 \times 10^{-13} e^{\frac{800}{T}}$ [BrO][CH_3O_2]	von Glasow et al. (2004)
BrO + NO	$\longrightarrow$	Br + NO_2	$8.7 \times 10^{-12} e^{\frac{260}{T}}$ [BrO][NO]	IUPAC
BrO + NO_2	$\longrightarrow$	$BrNO_3$	$\frac{k_0}{1+\frac{k_0}{k_\infty}} 0.6^{(1+\log_{10}(\frac{k_0}{k_\infty}))^{-1}}$ [BrO][NO_2] where: $k_0 = 5.2 \times 10^{-31} (\frac{T}{300})^{-3.2}$[M] $k_\infty = 6.9 \times 10^{-12} (\frac{T}{300})^{-2.9}$	IUPAC^A

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Table S4 – continued from previous page

Reactants		Products	Rate equation / s^{-1}	Reference
BrO + BrO	⟶	2 Br	2.7×10^{-12}[BrO][BrO]	IUPAC
BrO + BrO	⟶	Br_2	$2.9 \times 10^{-14} e^{\frac{840}{T}}$[BrO][BrO]	IUPAC
HBr + OH	⟶	Br + H_2O	$6.7 \times 10^{-12} e^{\frac{155}{T}}$[HBr][OH]	IUPAC
BrO + OH	⟶	Br + HO_2	$1.8 \times 10^{-11} e^{\frac{250}{T}}$[BrO][OH]	IUPAC
Br_2 + OH	⟶	HOBr + Br	$1.9 \times 10^{-11} e^{\frac{240}{T}}$[Br2][OH]	IUPAC
Br + NO_2	⟶	$BrNO_2$	$\frac{k_0}{1+\frac{k_0}{k_\infty}} 0.55^{(1+\log_{10}(\frac{k_0}{k_\infty}))^{-1}}$[Br][$NO_2$]	IUPAC
			where:	
			$k_0 = 4.2 \times 10^{-31} (\frac{T}{300})^{-2.4}$[M]	
			$k_\infty = 2.7 \times 10^{-11}$	
$BrNO_3$	⟶	BrO + NO_2	$2.8 \times 10^{13} e^{\frac{-12360}{T}}$[$BrNO_3$]	Orlando and Tyndall (1996)
Cl + O_3	⟶	ClO	$2.8 \times 10^{-11} e^{\frac{-250}{T}}$[Cl][$O_3$]	IUPAC
Cl + HO_2	⟶	0.8 HCl + 0.2 ClO + 0.2 OH	4.4×10^{-11}[Cl][H_2O_2]	IUPAC
Cl + H_2O_2	⟶	HCl	$1.1 \times 10^{-11} e^{\frac{-980}{T}}$[Cl][$H_2O_2$]	IUPAC
Cl + RO_2	⟶	0.5 ClO + 0.5 HCHO + 0.5 HO_2 + 0.5 HCl + 0.5 CO	1.6×10^{-10}[Cl][RO_2]	Burkholder et al. (2015)[B]
Cl + CH_4	⟶	HCl + CH_3O_2	$6.6 \times 10^{-12} e^{\frac{-1240}{T}}$[Cl][$CH_4$]	IUPAC
Cl + C_2H_6	⟶	HCl + RO_2	$7.1 \times 10^{-11} e^{\frac{-60}{T}}$[Cl][$C_2H_6$]	IUPAC
Cl + HCHO	⟶	HCl + HO_2 + CO	$8.1 \times 10^{-11} e^{\frac{-34}{T}}$[Cl][HCHO]	IUPAC
Cl + $ClNO_3$	⟶	Cl_2 + NO_3	$6.2 \times 10^{-12} e^{\frac{145}{T}}$[Cl][$ClNO_3$]	IUPAC
ClO + HO_2	⟶	HOCl	$2.2 \times 10^{-12} e^{\frac{340}{T}}$[ClO][$HO_2$]	IUPAC
ClO + CH_3O_2	⟶	Cl + HCHO + HO_2	$3.2 \times 10^{-12} e^{\frac{-110}{T}}$[ClO][$CH_3O_2$]	IUPAC[C]
ClO + NO	⟶	Cl + NO_2	$6.2 \times 10^{-12} e^{\frac{295}{T}}$[ClO][NO]	IUPAC
ClO + NO_2	⟶	$BrNO_2$	$\frac{k_0}{1+\frac{k_0}{k_\infty}} 0.4^{(1+\log_{10}(\frac{k_0}{k_\infty}))^{-1}}$[ClO][$NO_2$]	IUPAC
			where:	
			$k_0 = 1.6 \times 10^{-31} (\frac{T}{300})^{-3.4}$[M]	
			$k_\infty = 7.0 \times 10^{-11}$	
ClO + ClO	⟶	Cl_2	$1.0 \times 10^{-12} e^{\frac{-1590}{T}}$[ClO][ClO]	IUPAC
ClO + ClO	⟶	OClO + Cl	$3.5 \times 10^{-13} e^{\frac{-1370}{T}}$[ClO][ClO]	IUPAC
ClO + ClO	⟶	2 Cl	$3.0 \times 10^{-11} e^{\frac{-2450}{T}}$[ClO][ClO]	IUPAC

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Table S4 – continued from previous page

Reactants		Products	Rate equation / s^{-1}	Reference
HCl + OH	⟶	H_2O + Cl	$1.7 \times 10^{-12} e^{\frac{-230}{T}}$ [HCl][OH]	IUPAC
$ClNO_2$ + OH	⟶	HOCl + NO_2	$2.4 \times 10^{-12} e^{\frac{-1250}{T}}$ [$ClNO_2$][OH]	IUPAC
$ClNO_3$ + OH	⟶	0.5 ClO + 0.5 HNO_3 + 0.5 HOCl + 0.5 NO_3	$1.2 \times 10^{-12} e^{\frac{-330}{T}}$ [$ClNO_3$][OH]	IUPAC
BrO + ClO	⟶	Br + OClO	$1.6 \times 10^{-12} e^{\frac{430}{T}}$ [BrO][ClO]	IUPAC
BrO + ClO	⟶	BrCl	$5.8 \times 10^{-13} e^{\frac{170}{T}}$ [BrO][ClO]	IUPAC
BrO + ClO	⟶	Br + Cl	$2.9 \times 10^{-12} e^{\frac{220}{T}}$ [BrO][ClO]	IUPAC
Hg + Br	⟶	HgBr	$1.4 \times 10^{-32} (T/298)^{-1.86}$ [Hg][Br][M]	Horowitz et al. (2017)
Hg + Cl	⟶	HgCl	1.8×10^{-11} [Hg][Cl]	Sun et al. (2016)
HgBr + Br	⟶	$HgBr_2$	3.0×10^{-11} [HgBr][Br]	Horowitz et al. (2017)
HgBr + Cl	⟶	HgBrCl	$\frac{k_0}{1+\frac{k_0}{k_\infty}} 0.6^{(1+\log_{10}(\frac{k_0}{k_\infty}))^2}$ [HgBr][Cl] where: $k_0 = 2.27 \times 10^{-29} (\frac{T}{300})^{-4.37}$ [M] $k_\infty = 7.0 \times 10^{-11} (\frac{T}{300})^{-2.37}$	Horowitz et al. (2017)
HgCl + Br	⟶	HgBrCl	3.0×10^{-11} [HgCl][Br]	Horowitz et al. (2017)
HgCl + Cl	⟶	$HgCl_2$	$\frac{k_0}{1+\frac{k_0}{k_\infty}} 0.6^{(1+\log_{10}(\frac{k_0}{k_\infty}))^2}$ [HgBr][Cl]	Horowitz et al. (2017)
HgBr + Br	⟶	Hg + Br_2	3.9×10^{-11} [HgBr][Br]	Horowitz et al. (2017)
HgCl + Cl	⟶	Hg + Cl_2	$1.2 \times 10^{-11} e^{\frac{-5942}{T}}$ [HgCl][Cl]	Horowitz et al. (2017)
HgBr	⟶	Hg + Br	$1.6 \times 10^{-9} \frac{T}{298}^{-1.86} e^{\frac{-7801}{T}}$ [HgBr][M]	Horowitz et al. (2017)

A - for $F_c = 0.6$

B - rate of Cl + CH_3O_2 reaction

C - reaction channel 1 only

D - midpoint of narrowest range of rates in table 1 of Si and Ariya (2018)

References

Ammann, M., Cox, R. A., Crowley, J. N., Jenkin, M. E., Mellouki, A., Rossi, M. J., Troe, J., and Wallington, T. J.: Evaluated kinetic and photochemical data for atmospheric chemistry: Volume VI - heterogeneous reactions with liquid substrates, Atmospheric Chemistry and Physics, 13, 8045–8228, https://doi.org/10.5194/acp-13-8045-2013, 2013.

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Evaluated kinetic and photochemical data for atmospheric chemistry Volume I - gas phase reactions of O_x, HO_x, NO_x and SO_x species, Atmospheric Chemistry and Physics, 4, 1461–1738, https://doi.org/10.5194/acp-4-1461-2004, 2004.

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and IUPAC Subcommittee: Evaluated kinetic and photochemical data for atmospheric chemistry: Volume II - gas phase reactions of organic species, Atmospheric Chemistry and Physics, 6, 3625–4055, https://doi.org/10.5194/acp-6-3625-2006, 2006.

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Evaluated kinetic and photochemical data for atmospheric chemistry: Volume III - gas phase reactions of inorganic halogens, Atmospheric Chemistry and Physics, 7, 981–1191, https://doi.org/10.5194/acp-7-981-2007, 2007.

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and Wallington, T. J.: Evaluated kinetic and photochemical data for atmospheric chemistry: Volume IV - gas phase reactions of organic halogen species, Atmospheric Chemistry and Physics, 8, 4141–4496, https://doi.org/10.5194/acp-8-4141-2008, 2008.

Brimblecombe, P. and Clegg, S. L.: The solubility and behaviour of acid gases in the marine aerosol, Journal of Atmospheric Chemistry, 7, 1–18, https://doi.org/10.1007/bf00048251, 1988.

Brimblecombe, P. and Clegg, S. L.: Erratum, Journal of Atmospheric Chemistry, 8, 95, https://doi.org/10.1007/bf00053818, 1989.

Burkholder, J. B., Sander, S. P., Abbatt, J., Barker, J. R., Huie, R. E., Kolb, C. E., Kurylo, M. J., Orkin, V. L., Wilmouth, D. M., and H., W. P.: Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Evaluation No. 18, JPL Publication 15-10, http://jpldataeval.jpl.nasa.gov, 2015.

Crowley, J. N., Ammann, M., Cox, R. A., Hynes, R. G., Jenkin, M. E., Mellouki, A., Rossi, M. J., Troe, J., and Wallington, T. J.: Evaluated kinetic and photochemical data for atmospheric chemistry: Volume V - heterogeneous reactions on solid substrates, Atmospheric Chemistry and Physics, 10, 9059–9223, https://doi.org/10.5194/acp-10-9059-2010, 2010.

Horowitz, H. M., Jacob, D. J., Zhang, Y., Dibble, T. S., Slemr, F., Amos, H. M., Schmidt, J. A., Corbitt, E. S., Marais, E. A., and Sunderland, E. M.: A new mechanism for atmospheric mercury redox chemistry: implications for the global mercury budget, Atmospheric Chemistry and Physics, 17, 6353–6371, https://doi.org/10.5194/acp-17-6353-2017, 2017.

Jourdain, L., Roberts, T. J., Pirre, M., and Josse, B.: Modeling the reactive halogen plume from Ambrym and its impact on the troposphere with the CCATT-BRAMS mesoscale model, Atmospheric Chemistry and Physics, 16, 12 099–12 125, https://doi.org/10.5194/acp-16-12099-2016, 2016.

Marelle, L., Thomas, J. L., Ahmed, S., Tuite, K., Stutz, J., Dommergue, A., Simpson, W. R., Frey, M. M., and Baladima, F.: Implementation and impacts of surface and blowing snow sources of Arctic bromine activation within WRF-Chem 4.1.1, Journal of Advances in Modeling Earth Systems, p. e2020MS002391, https://doi.org/10.1029/2020MS002391, 2021.

Orlando, J. J. and Tyndall, G. S.: Rate Coefficients for the Thermal Decomposition of $BrONO_2$ and the Heat of Formation of $BrONO_2$, The Journal of Physical Chemistry, 100, 19 398–19 405, https://doi.org/10.1021/jp9620274, 1996.

Saiz-Lopez, A., Sitkiewicz, S. P., Roca-Sanjuán, D., Oliva-Enrich, J. M., Dávalos, J. Z., Notario, R., Jiskra, M., Xu, Y., Wang, F., Thackray, C. P., Sunderland, E. M., Jacob, D. J., Travnikov, O., Cuevas, C. A., Acuña, A. U., Rivero, D., Plane, J. M. C., Kinnison, D. E., and Sonke, J. E.: Photoreduction of gaseous oxidized mercury changes global atmospheric mercury speciation, transport and deposition, Nature Communications, 9, https://doi.org/10.1038/s41467-018-07075-3, 2018.

Saiz-Lopez, A., Acuña, A. U., Trabelsi, T., Carmona-García, J., Dávalos, J. Z., Rivero, D., Cuevas, C. A., Kinnison, D. E., Sitkiewicz, S. P., Roca-Sanjuán, D., and Francisco, J. S.: Gas-Phase Photolysis of Hg(I) Radical Species: A New Atmospheric Mercury Reduction Process, Journal of the American Chemical Society, 141, 8698–8702, https://doi.org/10.1021/jacs.9b02890, 2019.

Sander, R.: Compilation of Henry's law constants (version 4.0) for water as solvent, Atmospheric Chemistry and Physics, 15, 4399–4981, https://doi.org/10.5194/acp-15-4399-2015, 2015.

Si, L. and Ariya, P.: Recent Advances in Atmospheric Chemistry of Mercury, Atmosphere, 9, 76, https://doi.org/10.3390/atmos9020076, 2018.

Sun, G., Sommar, J., Feng, X., Lin, C.-J., Ge, M., Wang, W., Yin, R., Fu, X., and Shang, L.: Mass-Dependent and -Independent Fractionation of Mercury Isotope during Gas-Phase Oxidation of Elemental Mercury Vapor by Atomic Cl and Br, Environmental Science & Technology, 50, 9232–9241, https://doi.org/10.1021/acs.est.6b01668, 2016.

Tang, M. J., Cox, R. A., and Kalberer, M.: Compilation and evaluation of gas phase diffusion coefficients of reactive trace gases in the atmosphere: volume 1. Inorganic compounds, Atmospheric Chemistry and Physics, 14, 9233–9247, https://doi.org/10.5194/acp-14-9233-2014, 2014.

von Glasow, R., von Kuhlmann, R., Lawrence, M. G., Platt, U., and Crutzen, P. J.: Impact of reactive bromine chemistry in the troposphere, Atmospheric Chemistry and Physics, 4, 2481–2497, https://doi.org/10.5194/acp-4-2481-2004, 2004.

Wang, T. X., Kelley, M. D., Cooper, J. N., Beckwith, R. C., and Margerum, D. W.: Equilibrium, Kinetic, and UV-Spectral Characteristics of Aqueous Bromine Chloride, Bromine, and Chlorine Species, Inorganic Chemistry, 33, 5872–5878, https://doi.org/10.1021/ic00103a040, 1994.