Halogen activation in the plume of Masaya volcano: field observations and box model investigations

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Table S1: Gas species used in the HSC model and the mixing ratio of the atmospheric background composition taken from (Roberts et al., 2014).

Species	Mixing ratio	Species	Mixing ratio
H_2O(g)	-	Cl(g)	-
Ar(g)	0.0095	I(g)	-
N_2(g)	0.78	F(g)	-
O_2(g)	0.21	BrO(g)	-
CO_2(g)	0.0004	ClO(g)	-
CH_4(g)	1.70E-06	IO(g)	-
CO(g)	1.5E-07	O(g)	-
O_3(g)	6.40E-08	Cl_2(g)	-
OH(g)	6.90E-13	Br_2(g)	-
H_2O_2(g)	-	I_2(g)	-
HO_2(g)	3.00E-11	BrCl(g)	-
NO(g)	5.00E-11	HOCl(g)	-
NO_2(g)	1.10E-10	H_2(g)	-
HNO_2(g)	-	H(g)	-
NO_3(g)	5.00E-14	H_2SO_4(g)	-
HNO_3(g)	-	N_2O(g)	-
N_2O_5(g)	-	HNO(g)	-
CH_3OH(g)	-	OClO(g)	-
SO_2(g)	-	HF(g)	-
HCl(g)	-	HI(g)	-
HBr(g)	-	Br(g)	-

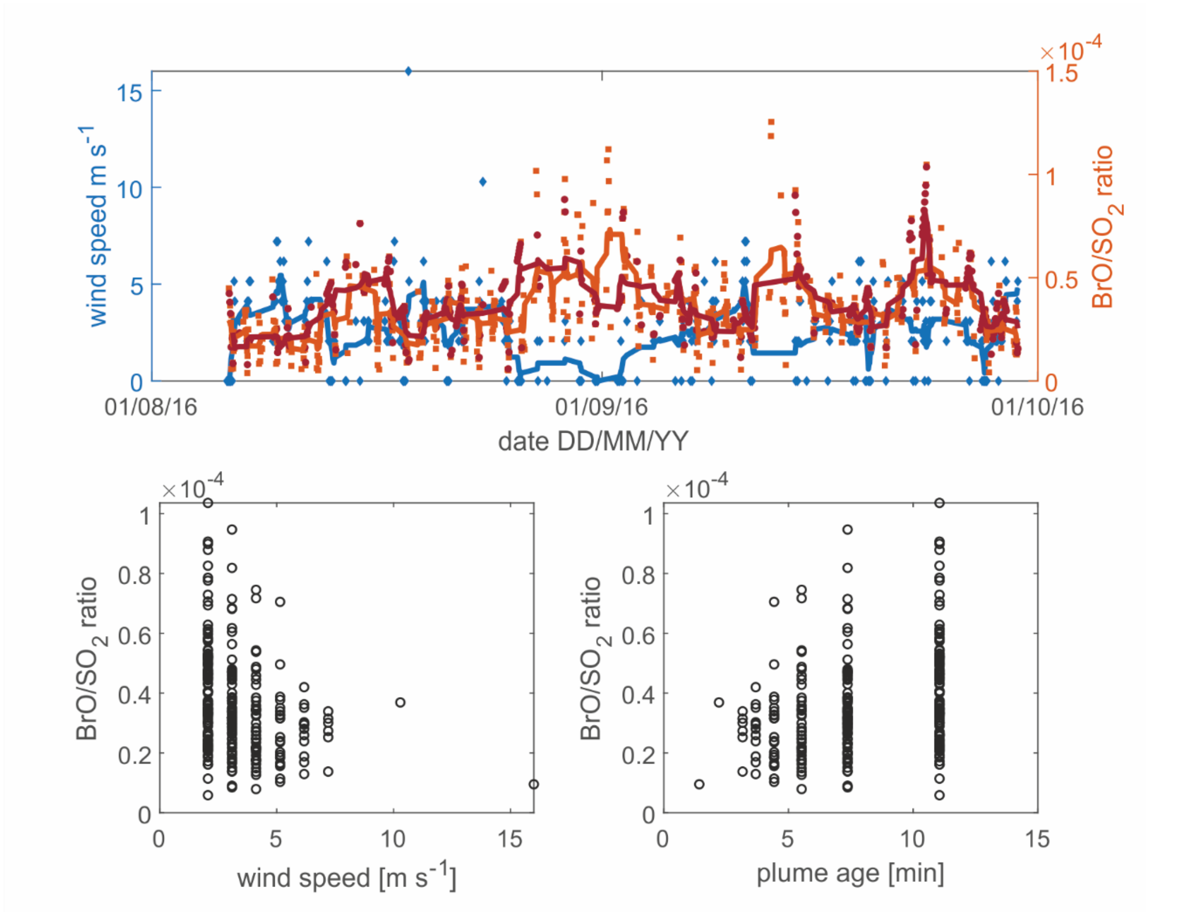


Figure S1: (a) Wind speed at the meteorological measurement station at Managua airport (blue) and BrO/SO_2 mixing ratios at Masaya volcano (orange) and interpolated BrO/SO_2 mixing ratios (red) at the time of wind speed measurements; (b) BrO/SO_2 mixing ratio vs. wind speed and (c) BrO/SO_2 mixing ratio vs. estimated plume age

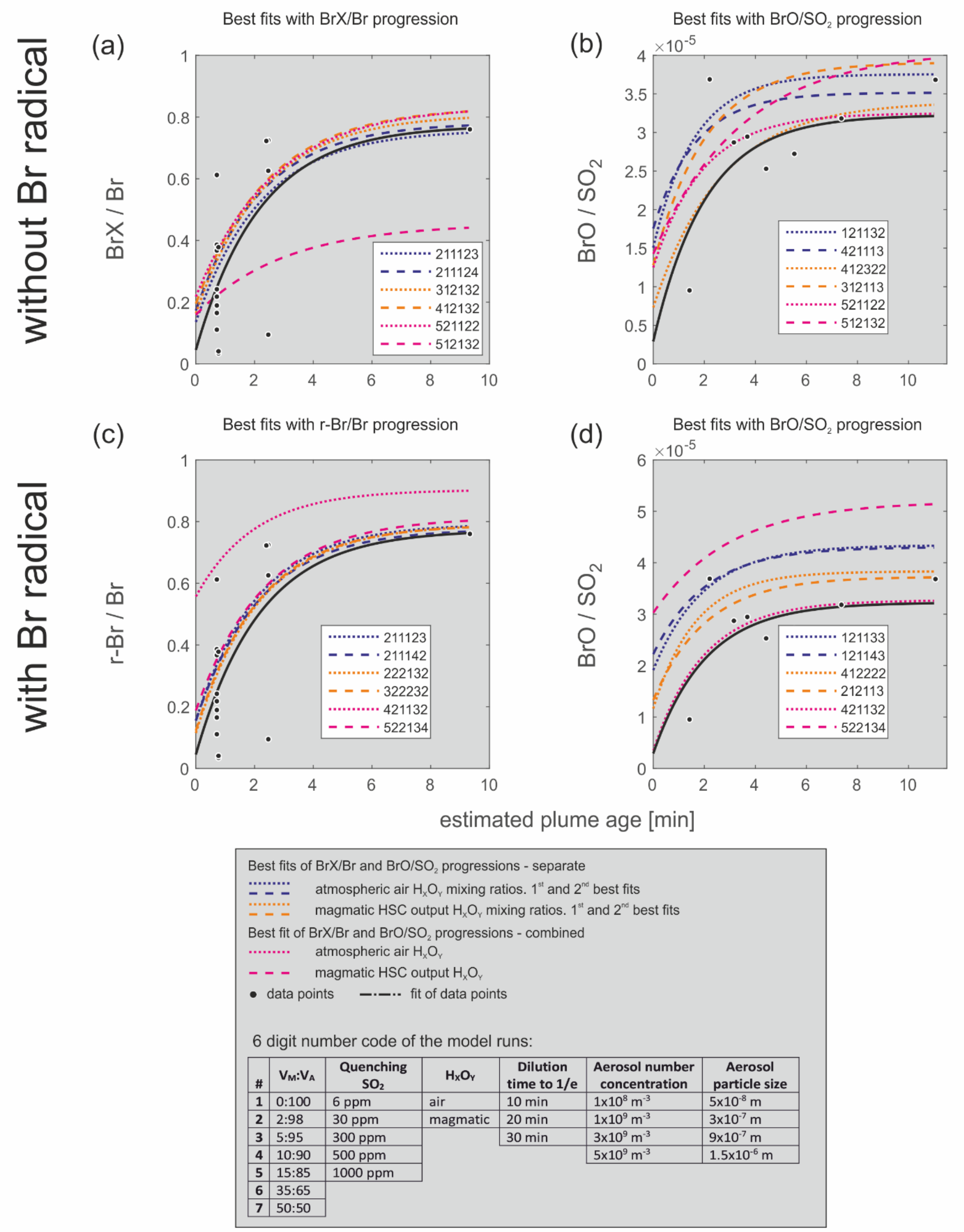
Selection of model scenarios to compare with field measurements

Multiple model runs were performed to further study the chemistry in volcanic plumes and investigate whether the field observations can be reproduced by theoretical predictions. For this, a combination of HSC high-temperature model and CAABA/MECCA atmospheric box model as explained in the text of the paper.

In order to simplify the selection of model scenarios that fit best with the observations, a computational procedure was chosen that compares the fit of model results for the progression of selected ratios (e.g. BrX/Br or BrO/SO_2) with the fit of the respective field measurements data. To do so the data was fitted by a function that produces the shape of the progression in a way that it increases the ratios from low values (virtually zero) at the start of the model run to a specific value (e.g. 0.76 for BrX/Br) at the plume age corresponding to the distance of the farthest sample location (2.8 km or approx. 9.3 minutes). For this, an exponential function was applied given by equation (1), with c being the average ratio measured (or modelled) at a distance of about 2.8 km or corresponding plume age:

$$f(x) = a * exp(-b * x) + c \qquad \text{(Eq. 1)}$$

Figure S2 shows the selected model progressions with the corresponding measurement data.



#	$V_M:V_A$	Quenching SO_2	H_XO_Y	Dilution time to 1/e	Aerosol number concentration	Aerosol particle size
1	0:100	6 ppm	air	10 min	1×10^{8} m^{-3}	5×10^{-8} m
2	2:98	30 ppm	magmatic	20 min	1×10^{9} m^{-3}	3×10^{-7} m
3	5:95	300 ppm		30 min	3×10^{9} m^{-3}	9×10^{-7} m
4	10:90	500 ppm			5×10^{9} m^{-3}	1.5×10^{-6} m
5	15:85	1000 ppm				
6	35:65					
7	50:50					

Figure S2: (a) BrX/Br samples (black circles), fit through the sample data points using *f(x) = a*exp(-b*x) + c* (Eq. 1, see text) as a fit function (black line), fits of the closest model runs see description in legend (modelled BrX includes: Br_2, BrCl, $BrNO_2$, $BrNO_3$, HOBr and BrO), (b) BrO/SO_2 median values for different plume ages and fits through measurement and model data using Eq. 1 similar to (a), (c) and (d) similar procedure as in (a) and (b), but modelled reactive Br species (r-Br) also include Br radicals.

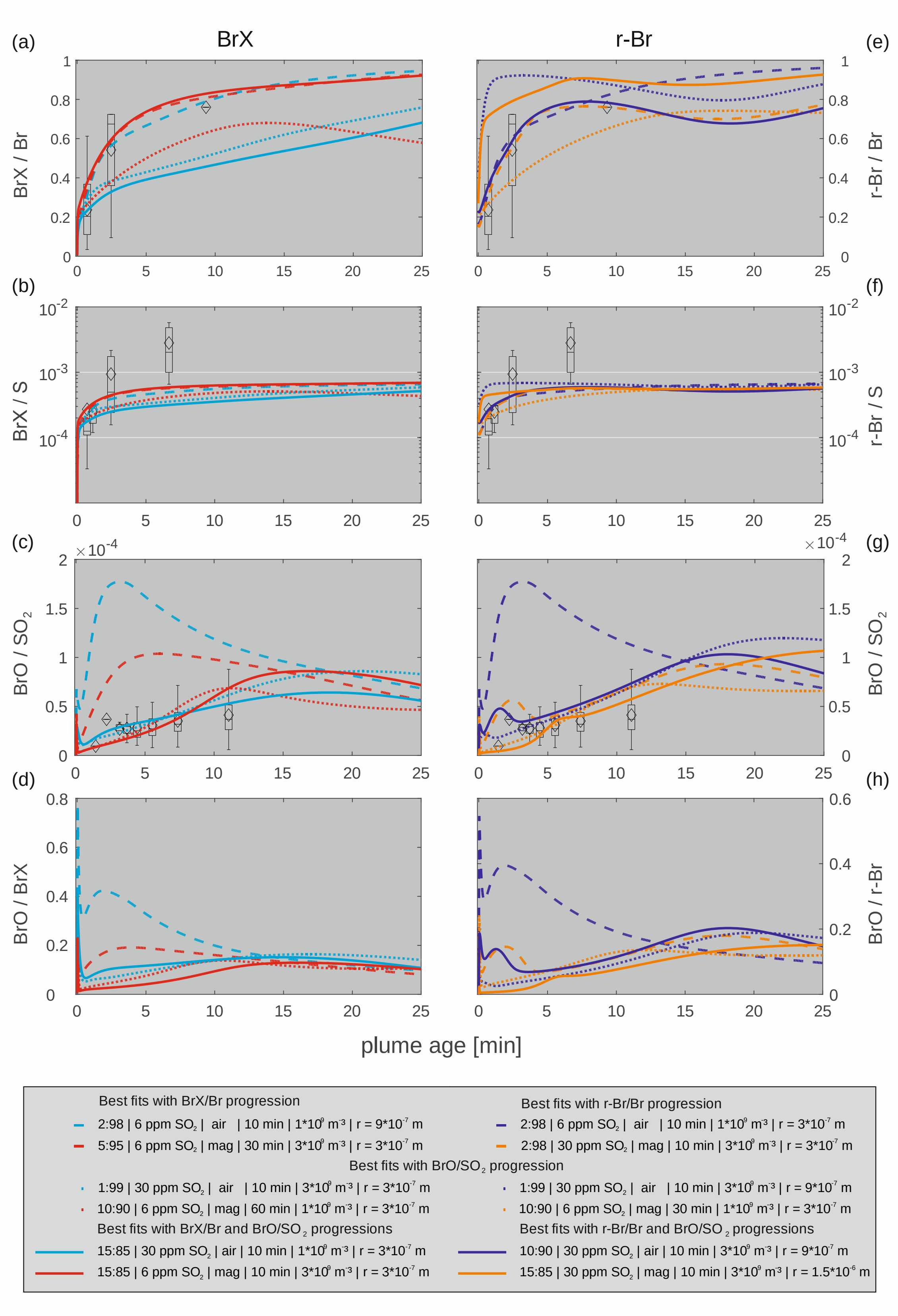


Figure S3: Temporal evolution of different modelled bromine species ratios (molar) over the model time of 25 minutes with the respective measurement data (if available). Each sub figure shows the model runs that are closest to the measurement data, derived by the fit comparison approach described in section Fehler! Verweisquelle konnte nicht gefunden werden.**. The legend provides the detailed model parameter ensembles for the respective plots. This figure is a supplemented version of Figure 6 providing the best fitting model runs r-Br/Br and BrX/Br.**

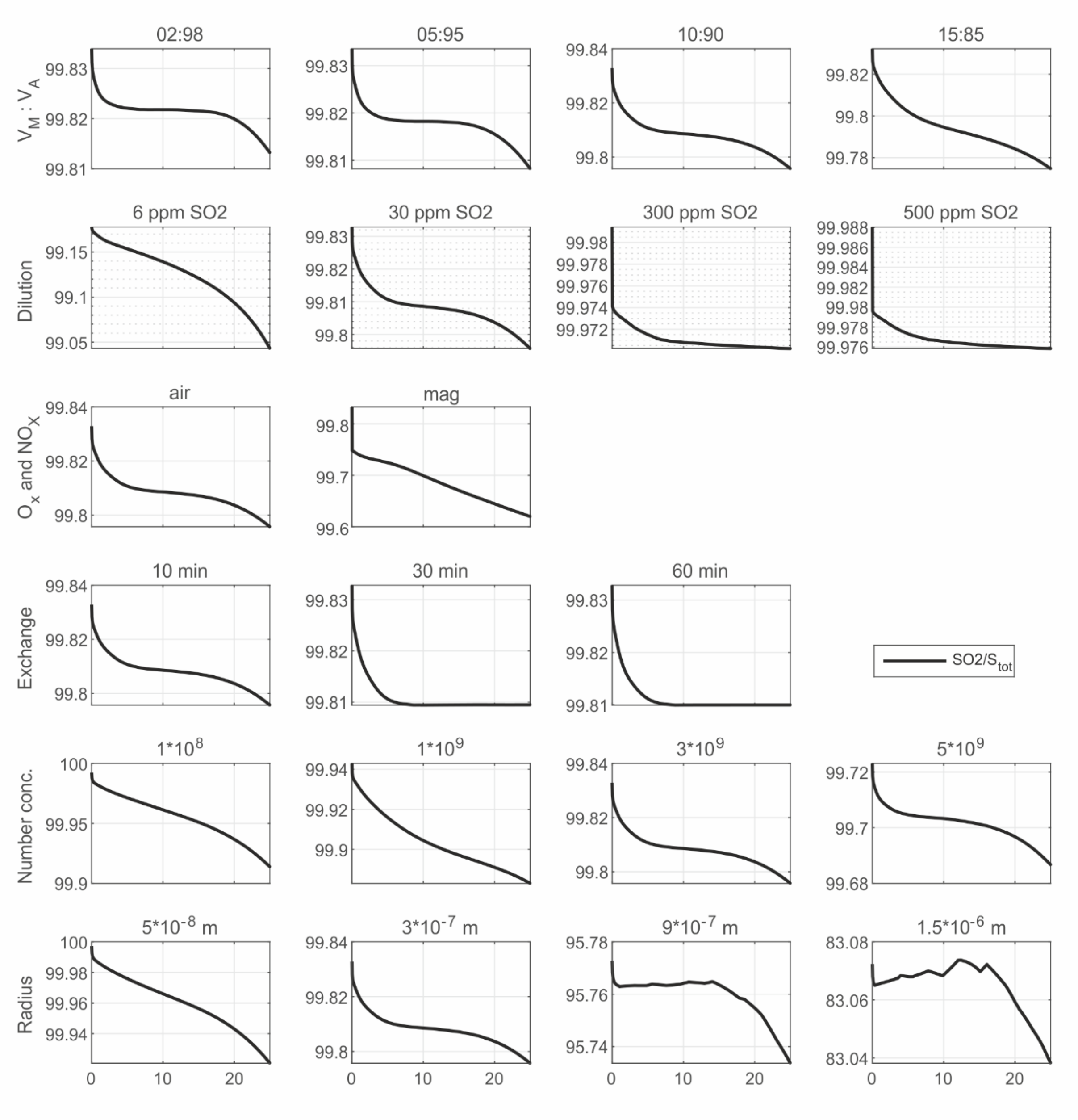


Figure S4: SO_2 over total sulfur for selected CAABA/MECCA model runs corresponding to Figure 8. Variations of the base run by changes of one parameter (horizontal rows).

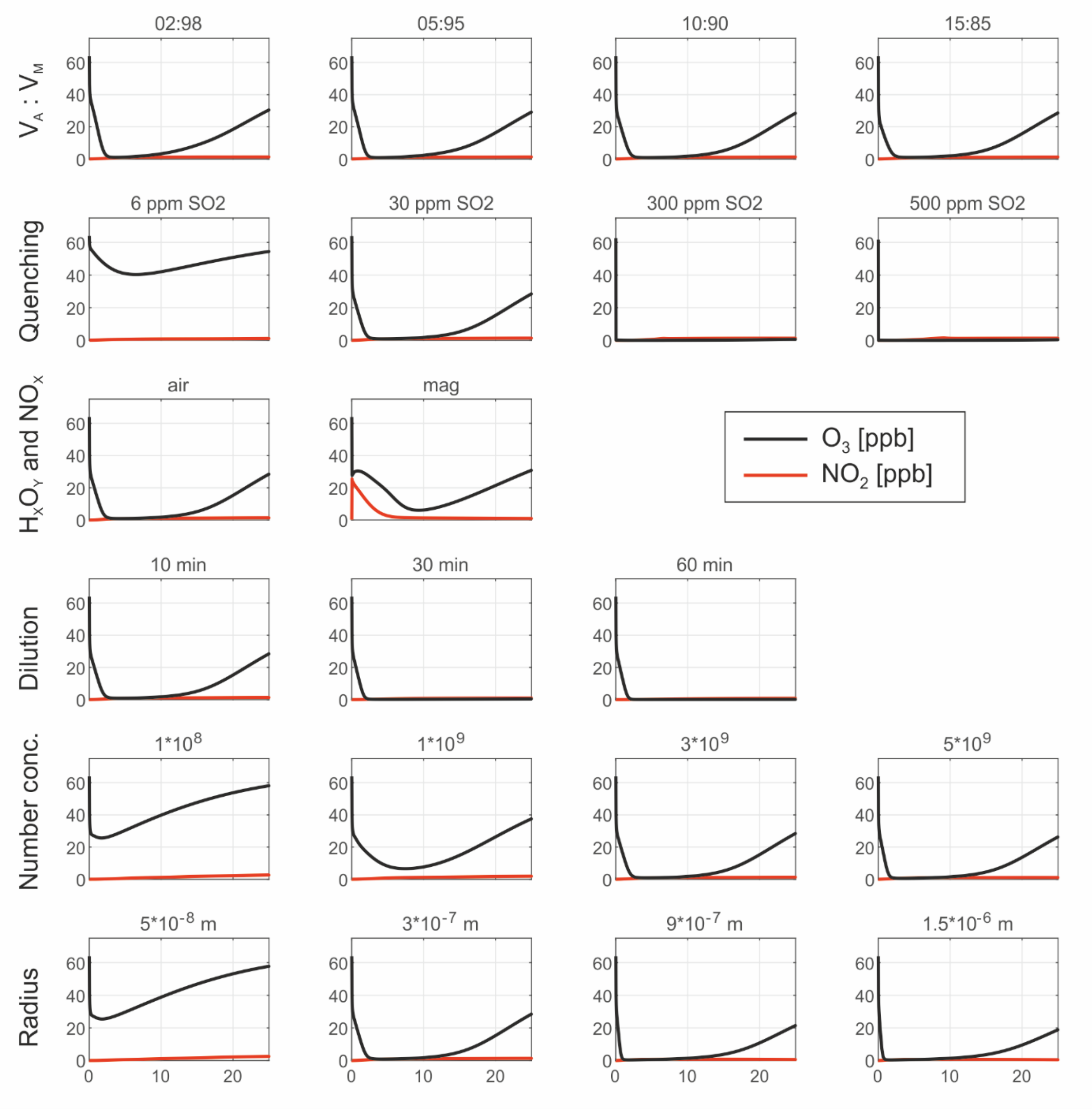


Figure S5: O_3 and NO_2 mixing ratios during the model runs in Figure 8. Variations of the base run by changes of one parameter (horizontal rows)

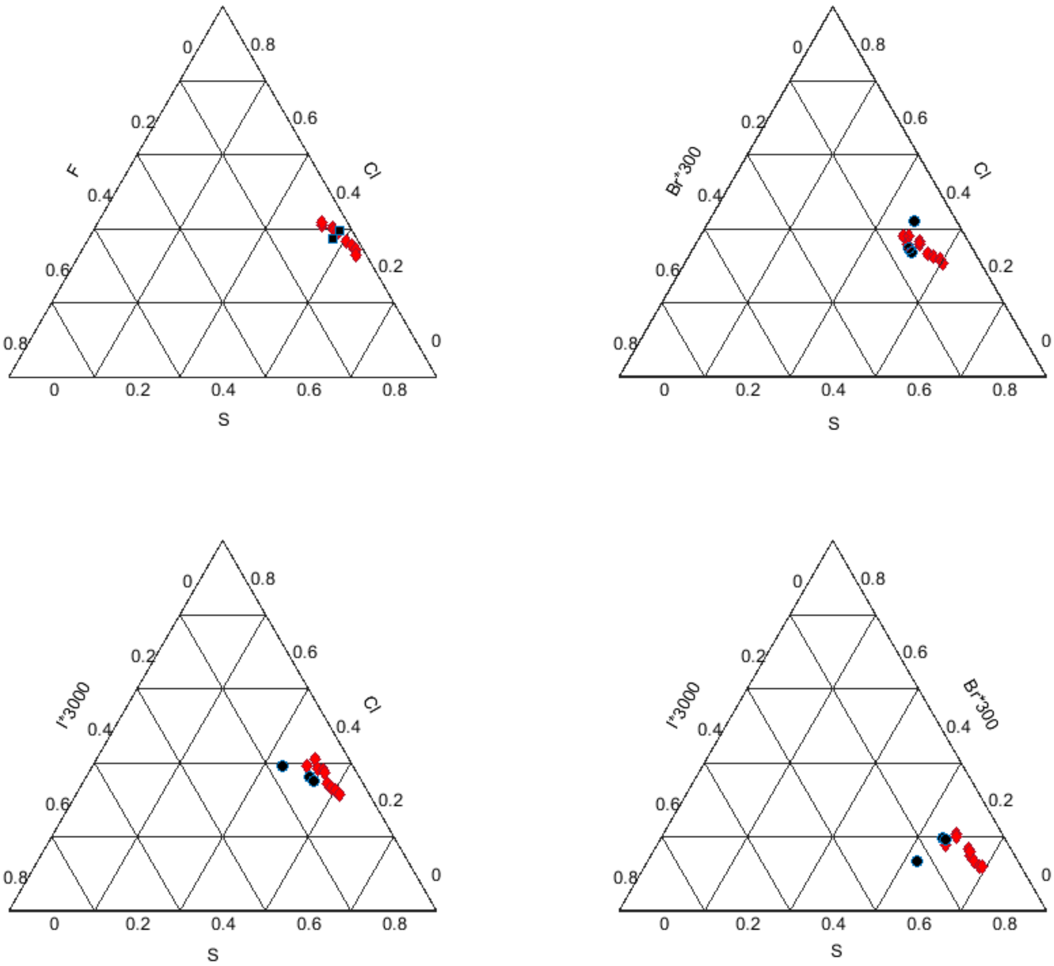


Figure S6: Ternary plots of Halogen to Sulfur ratios; red diamonds: July samples, black circles: September samples

Table S2: Results of denuder, alkaline and electrochemical sensor measurements (G = ground, R = Raschig tube, D = Drechsel bottle, UAV = unmanned aerial vehicle, Type 1 = 1 M NaOH, 4 = 4 M NaOH). HalX (e.g., Br_2, Cl_2 or BrCl) mixing ratios were derived from denuder samples with known volume of sampled plume gas; for certain alkaline trap samples the sampled volume is unknown and only a ratio of the respective halogen to sulfur was calculated from sample concentrations.

No.	Date	Type	Location	Distance [m]	S (SO_2) [ppm]	F [ppm]	F/S	Cl [ppm]	Cl/S	ClX [ppb]	ClX/S	ClX/Cl	Br_Y [ppb]	Br/S	BrX [ppb]	BrX/S	BrX/Br	I [ppb]	I/S	IX [ppb]	IX/S	IX/I
1	14.07.2016	GR 1	Lookout (s)	231 ± 20	4.18 ± 0.22	0.12 ± 0.01	1.6E-01 ± 1.2E-02	3.24 ± 0.17	0.77 ± 0.06				3.72 ± 0.07	8.89E-04 ± 4.95E-05				0.30 ± 0.07	7.2E-05 ± 1.8E-05			
2	14.07.2016	GD 1	Pole	214 ± 20	0.71 ± 0.04		1.1E-01 ± 8.1E-03	0.53 ± 0.03	0.75 ± 0.06	0.17 ± 0.24	2.4E-04 ± 3.4E-04	3.2E-04 ± 4.6E-04	1.11 ± 0.06	1.57E-03 ± 1.14E-04	0.68 ± 0.15	9.6E-04 ± 2.2E-04	0.61 ± 0.14	0.06 ± 0.06	8.5E-05 ± 7.9E-05	0.11 ± 0.01	1.6E-04 ± 2.0E-05	
3	14.07.2016	GR 1	Pole	214 ± 20		0.15 ± 0.01	1.8E-01 ± 1.3E-02	2.83 ± 0.15	0.80 ± 0.06				3.54 ± 0.06	1.00E-03 ± 5.48E-05				0.18 ± 0.06	5.2E-05 ± 1.7E-05			
4	14.07.2016	GD 1	Pole	214 ± 20	0.83 ± 0.04		5.6E-02 ± 4.0E-03	0.63 ± 0.03	0.76 ± 0.06	0.17 ± 0.24	2.1E-04 ± 3.0E-04	2.7E-04 ± 3.9E-04	1.85 ± 0.08	2.24E-03 ± 1.50E-04	0.68 ± 0.15	8.2E-04 ± 1.9E-04	0.37 ± 0.08	0.05 ± 0.08	5.6E-05 ± 9.5E-05	0.11 ± 0.01	1.4E-04 ± 1.7E-05	
5	14.07.2016	GD 4	Pole	214 ± 20		0.52 ± 0.03	1.2E-01 ± 8.8E-03		0.90 ± 0.06					5.46E-04 ± 3.02E-05					6.2E-05 ± 7.4E-06			
6	15.07.2016	GR 1	Nindirí Rim	740 ± 50	1.13 ± 0.06	0.34 ± 0.02	3.8E-02 ± 2.7E-03	0.54 ± 0.03	0.48 ± 0.04	0.73 ± 0.18	6.5E-04 ± 1.6E-04	1.3E-03 ± 3.3E-04	0.77 ± 0.03	6.86E-04 ± 4.71E-05	0.56 ± 0.10	5.0E-04 ± 8.9E-05	0.72 ± 0.13	0.05 ± 0.03	4.7E-05 ± 3.1E-05	0.07 ± 0.01	5.9E-05 ± 7.0E-06	
7	15.07.2016	GR 1	Pole	214 ± 20	8.81 ± 0.46		1.0E-01 ± 7.1E-03	4.45 ± 0.23	0.51 ± 0.04	0.26 ± 0.26	3.0E-05 ± 3.0E-05	5.9E-05 ± 5.9E-05	4.44 ± 0.08	5.04E-04 ± 2.76E-05	1.71 ± 0.19	1.9E-04 ± 2.4E-05	0.39 ± 0.04	0.33 ± 0.08	3.8E-05 ± 8.8E-06	0.17 ± 0.02	1.9E-05 ± 2.1E-06	0.51 ± 0.13
8	15.07.2016	GD 4	Pole	214 ± 20			7.9E-02 ± 5.6E-03		0.72 ± 0.05					8.79E-04 ± 8.08E-05					7.2E-05 ± 2.5E-05			
9	15.07.2016	GD 4	Pole	214 ± 20					0.84 ± 0.06					7.74E-04 ± 4.32E-05					4.0E-05 ± 2.7E-06			
10	16.07.2016	GR 1	Nindirí Rim	740 ± 50	0.98 ± 0.05	0.37 ± 0.02	4.9E-02 ± 3.5E-03	1.32 ± 0.07	1.35 ± 0.10				1.62 ± 0.04	1.66E-03 ± 9.65E-05	0.15 ± 0.07	1.6E-04 ± 6.8E-05	0.09 ± 0.04	0.09 ± 0.04	9.6E-05 ± 4.3E-05	0.03 ± 0.00	2.6E-05 ± 4.3E-06	0.27 ± 0.13
11	16.07.2016	GR 1	Pole	214 ± 20	7.56 ± 0.39			4.54 ± 0.24	0.60 ± 0.04				4.97 ± 0.10	6.57E-04 ± 3.66E-05				0.36 ± 0.10	4.7E-05 ± 1.3E-05			
12	17.07.2016	UAV	Caldera Valley	1989 ± 100	1.92 ± 0.09										1.26 ± 0.69	6.6E-04 ± 3.6E-04				0.18 ± 0.04	9.5E-05 ± 2.2E-05	
13	18.07.2016	GR 1	Nindirí Rim	740 ± 50	0.74 ± 0.04	0.10 ± 0.01	2.7E-02 ± 1.9E-03	1.70 ± 0.09	2.30 ± 0.17				1.31 ± 0.03	1.78E-03 ± 9.89E-05				0.05 ± 0.03	6.9E-05 ± 3.5E-05	0.03 ± 0.00	3.9E-05 ± 5.2E-06	0.57 ± 0.30
14	18.07.2016	GR 1	Pole	214 ± 20	3.61 ± 0.19			1.95 ± 0.10	0.54 ± 0.04				1.85 ± 0.04	5.11E-04 ± 2.86E-05	0.45 ± 0.06	1.2E-04 ± 1.7E-05	0.24 ± 0.03	0.15 ± 0.04	4.2E-05 ± 1.1E-05	0.09 ± 0.00	2.6E-05 ± 1.5E-06	0.62 ± 0.15
15	20.07.2016	GR 1	Pole	214 ± 20	2.65 ± 0.14	0.09 ± 0.01	3.3E-02 ± 2.3E-03	1.51 ± 0.08	0.57 ± 0.04				1.55 ± 0.03	5.84E-04 ± 3.28E-05	0.34 ± 0.05	1.3E-04 ± 2.1E-05	0.22 ± 0.03	0.12 ± 0.03	4.5E-05 ± 1.3E-05	0.08 ± 0.01	3.1E-05 ± 2.6E-06	0.70 ± 0.20
16	20.07.2016	GR 1	Nindirí Rim	740 ± 50	0.96 ± 0.05			0.89 ± 0.05	0.93 ± 0.07				1.22 ± 0.03	1.28E-03 ± 7.30E-05				0.06 ± 0.03	6.6E-05 ± 3.0E-05	0.02 ± 0.00	2.0E-05 ± 3.0E-06	0.31 ± 0.15
17	20.07.2016	UAV	Caldera Valley	1896 ± 100	0.51 ± 0.05										2.91 ± 0.75	5.7E-03 ± 1.6E-03				0.08 ± 0.03	1.5E-04 ± 6.4E-05	
18	20.07.2016	UAV	Caldera Valley	2122 ± 100	0.59 ± 0.05										1.19 ± 0.62	2.0E-03 ± 1.1E-03				0.06 ± 0.03	1.1E-04 ± 5.1E-05	
19	21.07.2016	GR 1	Nindirí Rim	740 ± 50	2.74 ± 0.14	0.29 ± 0.01	7.0E-02 ± 5.0E-03	2.00 ± 0.10	0.73 ± 0.05				2.56 ± 0.06	9.33E-04 ± 5.27E-05				0.17 ± 0.06	6.3E-05 ± 2.1E-05			
20	21.07.2016	GR 1	Nindirí Rim	740 ± 50	1.61 ± 0.08	0.56 ± 0.03	7.3E-02 ± 5.1E-03	1.46 ± 0.08	0.91 ± 0.07				1.81 ± 0.04	1.12E-03 ± 6.34E-05				0.09 ± 0.04	5.7E-05 ± 2.5E-05			
21	21.07.2016	GR 1	Pole	214 ± 20	4.06 ± 0.21		1.1E-01 ± 8.1E-03	2.76 ± 0.14	0.68 ± 0.05				3.05 ± 0.05	7.52E-04 ± 4.10E-05				0.19 ± 0.05	4.6E-05 ± 1.2E-05			
22	21.07.2016	GR 1	Pole	214 ± 20	7.67 ± 0.40		1.1E-01 ± 7.5E-03	5.36 ± 0.28	0.70 ± 0.05				5.57 ± 0.55	7.26E-04 ± 8.07E-05	0.92 ± 0.08	1.2E-04 ± 1.2E-05	0.17 ± 0.02	0.34 ± 0.55	4.4E-05 ± 7.1E-05	0.11 ± 0.01	1.4E-05 ± 1.2E-06	0.32 ± 0.52
23	21.07.2016	GD 1	Pole	214 ± 20		0.20 ± 0.01	7.4E-02 ± 5.2E-03		0.63 ± 0.04					6.16E-04 ± 3.09E-05					4.9E-05 ± 2.5E-06			
24	21.07.2016	GD 1	Pole	214 ± 20		0.14 ± 0.01	8.4E-02 ± 6.0E-03		0.84 ± 0.06					1.24E-03 ± 6.86E-05					9.2E-05 ± 4.8E-06			
25	22.07.2016	GR 1	Lookout (s)	231 ± 20	6.01 ± 0.31	0.46 ± 0.02	7.6E-02 ± 5.4E-03	4.34 ± 0.23	0.72 ± 0.05				5.86 ± 0.11	9.75E-04 ± 5.38E-05	0.20 ± 0.07	3.3E-05 ± 1.1E-05	0.03 ± 0.01	0.32 ± 0.11	5.3E-05 ± 1.8E-05	0.05 ± 0.01	8.7E-06 ± 1.0E-06	0.16 ± 0.06
26	22.07.2016	GR 1	Lookout (s)	231 ± 20	6.01 ± 0.31			4.34 ± 0.23	0.72 ± 0.05				5.86 ± 0.11	9.75E-04 ± 5.38E-05	0.24 ± 0.07	4.0E-05 ± 1.2E-05	0.04 ± 0.01	0.32 ± 0.11	5.3E-05 ± 1.8E-05	0.06 ± 0.01	1.0E-05 ± 1.1E-06	0.19 ± 0.07
27	01.09.2016	GR 1	Pole	214 ± 20	5.16 ± 0.27	0.52 ± 0.03	1.0E-01 ± 7.2E-03	3.35 ± 0.17	0.65 ± 0.05	1.16 ± 0.21	2.2E-04 ± 4.3E-05	3.5E-04 ± 6.5E-05	4.97 ± 0.08	9.63E-04 ± 5.27E-05	0.94 ± 0.10	1.8E-04 ± 2.2E-05	0.19 ± 0.02	0.36 ± 0.08	7.0E-05 ± 1.7E-05	0.12 ± 0.01	2.3E-05 ± 2.1E-06	0.32 ± 0.08
28	02.09.2016	GR 1	San Pedro Rim	720 ± 50						0.07 ± 0.10			0.35 ± 0.02		0.26 ± 0.05		0.72 ± 0.14	0.05 ± 0.02				0.75 ± 0.29
29	03.09.2016	GR 1	Nindirí Rim	740 ± 50	0.22 ± 0.01	0.17 ± 0.01	5.0E-02 ± 3.6E-03	0.64 ± 0.03	2.94 ± 0.22	0.55 ± 0.12	2.5E-03 ± 5.7E-04	8.5E-04 ± 1.9E-04	0.75 ± 0.02	3.45E-03 ± 2.07E-04	0.47 ± 0.06	2.2E-03 ± 3.0E-04	0.63 ± 0.08	0.05 ± 0.02	2.4E-04 ± 1.0E-04	0.01 ± 0.00	4.0E-05 ± 1.2E-05	0.17 ± 0.09
30	03.09.2016	GR 1	Pole	214 ± 20	3.31 ± 0.17			2.27 ± 0.12	0.69 ± 0.05	0.20 ± 0.12	6.1E-05 ± 3.7E-05	8.9E-05 ± 5.4E-05	3.27 ± 0.26	9.89E-04 ± 9.28E-05	0.36 ± 0.06	1.1E-04 ± 2.0E-05	0.11 ± 0.02	0.24 ± 0.26	7.3E-05 ± 7.7E-05	0.06 ± 0.00	1.9E-05 ± 1.8E-06	0.25 ± 0.27
31	03.09.2016	UAV	Nindirí Crater	351 ± 50	3.32 ± 0.14					1.42 ± 1.71	4.3E-04 ± 5.2E-04				1.04 ± 0.76	3.1E-04 ± 2.3E-04						
32	03.09.2016	UAV	Nindirí Crater	337 ± 50	11.04 ± 0.29					2.48 ± 1.35	2.2E-04 ± 1.2E-04				3.36 ± 0.77	3.0E-04 ± 7.0E-05				0.11 ± 0.03	9.8E-06 ± 2.8E-06	
33	03.09.2016	UAV	Nindirí Crater	337 ± 50	11.04 ± 0.29										1.32 ± 0.55	1.2E-04 ± 5.0E-05				0.13 ± 0.03	1.1E-05 ± 2.8E-06	
34	04.09.2016	GR 1	Nindirí Rim	740 ± 50	0.31 ± 0.02			1.02 ± 0.05	3.27 ± 0.24				1.08 ± 0.02	3.45E-03 ± 1.88E-04				0.05 ± 0.02	1.6E-04 ± 5.7E-05			
35	04.09.2016	GR 1	Lookout (night)	231 ± 20	0.85 ± 0.04			0.75 ± 0.04	0.88 ± 0.06	7.58 ± 0.83	8.9E-03 ± 1.1E-03	1.0E-02 ± 1.2E-03	0.60 ± 0.06	7.01E-04 ± 7.59E-05	0.23 ± 0.07	2.7E-04 ± 8.7E-05	0.38 ± 0.13	0.11 ± 0.06	1.2E-04 ± 6.7E-05	0.04 ± 0.00	4.3E-05 ± 5.5E-06	0.35 ± 0.19
36	05.09.2016	GR 1	Cerro Ventarrón	2800 ± 200						0.75 ± 0.13			0.29 ± 0.02		0.22 ± 0.05		0.76 ± 0.20	0.03 ± 0.02		0.02 ± 0.00		0.92 ± 0.67

Table S3: Overview on the HSC output and species and their mixing ratios at different volume ratios of atmospheric and magmatic gas at 1000°C

Temperature	1000°C							
VA:VM	0:100	1:99	2:98	5:95	10:90	15:85	35:65	50:50
H2O(g)	9.30E-01	9.21E-01	9.11E-01	8.83E-01	8.37E-01	7.90E-01	3.25E-01	4.65E-01
N2(g)	0.00E+00	7.80E-03	1.56E-02	3.90E-02	7.80E-02	1.17E-01	5.07E-01	3.90E-01
O2(g)	6.43E-06	2.04E-03	4.12E-03	1.04E-02	2.08E-02	3.13E-02	1.37E-01	1.05E-01
CO2(g)	4.39E-02	4.34E-02	4.30E-02	4.17E-02	3.95E-02	3.74E-02	1.56E-02	2.21E-02
CH4(g)	1.37E-24	1.32E-29	3.14E-30	4.52E-31	9.53E-32	3.56E-32	1.32E-34	6.51E-34
CO(g)	1.53E-06	8.48E-08	5.92E-08	3.62E-08	2.42E-08	1.87E-08	3.73E-09	6.04E-09
O3(g)	6.55E-18	3.72E-14	1.07E-13	4.25E-13	1.21E-12	2.23E-12	2.03E-11	1.36E-11
CH3OH(g)	1.14E-24	1.95E-28	6.61E-29	1.51E-29	4.51E-30	2.07E-30	1.60E-32	6.91E-32
SO2(g)	1.49E-02	1.47E-02	1.45E-02	1.40E-02	1.31E-02	1.24E-02	4.95E-03	7.12E-03
HCl(g)	1.03E-02	1.02E-02	1.01E-02	9.76E-03	9.25E-03	8.73E-03	3.59E-03	5.13E-03
HBr(g)	1.06E-05	9.11E-06	8.75E-06	8.07E-06	7.24E-06	6.59E-06	1.98E-06	3.16E-06
HF(g)	1.05E-03	1.04E-03	1.03E-03	9.99E-04	9.46E-04	8.93E-04	3.68E-04	5.26E-04
HI(g)	3.22E-08	7.64E-09	6.30E-09	4.76E-09	3.67E-09	3.03E-09	5.58E-10	1.01E-09
Br(g)	4.77E-07	1.75E-06	2.01E-06	2.37E-06	2.61E-06	2.70E-06	1.83E-06	2.28E-06
Cl(g)	1.42E-06	5.95E-06	7.06E-06	8.74E-06	1.01E-05	1.09E-05	1.01E-05	1.13E-05
I(g)	6.57E-07	6.62E-07	6.54E-07	6.31E-07	5.95E-07	5.60E-07	2.33E-07	3.30E-07
F(g)	6.34E-13	2.66E-12	3.16E-12	3.92E-12	4.54E-12	4.88E-12	4.53E-12	5.07E-12
BrO(g)	1.66E-12	1.09E-10	1.78E-10	3.33E-10	5.17E-10	6.58E-10	9.29E-10	1.02E-09
ClO(g)	1.13E-10	8.45E-09	1.43E-08	2.80E-08	4.59E-08	6.05E-08	1.17E-07	1.15E-07
IO(g)	1.39E-12	2.49E-11	3.49E-11	5.35E-11	7.14E-11	8.25E-11	7.15E-11	8.89E-11
Cl2(g)	2.12E-08	3.75E-07	5.28E-07	8.09E-07	1.09E-06	1.26E-06	1.08E-06	1.35E-06
Br2(g)	4.34E-11	5.84E-10	7.71E-10	1.07E-09	1.29E-09	1.39E-09	6.35E-10	9.92E-10
I2(g)	2.62E-12	2.65E-12	2.59E-12	2.41E-12	2.14E-12	1.90E-12	3.27E-13	6.60E-13
BrCl(g)	2.05E-09	3.16E-08	4.31E-08	6.30E-08	8.01E-08	8.93E-08	5.59E-08	7.81E-08
HOCl(g)	6.56E-09	1.16E-07	1.63E-07	2.50E-07	3.36E-07	3.89E-07	3.34E-07	4.17E-07
H2(g)	1.91E-05	1.06E-06	7.41E-07	4.52E-07	3.03E-07	2.33E-07	4.59E-08	7.50E-08
H(g)	3.16E-09	7.44E-10	6.21E-10	4.86E-10	3.97E-10	3.49E-10	1.55E-10	1.98E-10
H2SO4(g)	7.94E-09	1.38E-07	1.91E-07	2.84E-07	3.58E-07	3.91E-07	1.34E-07	2.42E-07
OClO(g)	9.98E-14	9.27E-14	2.22E-13	6.92E-13	1.61E-12	2.60E-12	1.05E-11	8.99E-12
OH(g)	1.73E-06	7.27E-06	8.62E-06	1.07E-05	1.24E-05	1.33E-05	1.24E-05	1.38E-05
H2O2(g)	1.06E-10	1.87E-09	2.63E-09	4.04E-09	5.42E-09	6.28E-09	5.39E-09	6.75E-09
HO2(g)	9.80E-11	7.34E-09	1.24E-08	2.43E-08	3.99E-08	5.27E-08	1.02E-07	9.99E-08
O(g)	2.73E-10	4.88E-09	6.93E-09	1.10E-08	1.56E-08	1.91E-08	3.99E-08	3.49E-08
NO(g)	0.00E+00	3.56E-06	7.15E-06	1.79E-05	3.59E-05	5.40E-05	2.35E-04	1.80E-04
NO2(g)	0.00E+00	4.34E-09	1.24E-08	4.93E-08	1.40E-07	2.58E-07	2.34E-06	1.57E-06
NO3(g)	0.00E+00	1.30E-16	5.29E-16	3.34E-15	1.34E-14	3.03E-14	5.75E-13	3.38E-13
HNO3(g)	0.00E+00	5.18E-14	1.75E-13	8.66E-13	2.85E-12	5.64E-12	4.75E-11	3.57E-11
N2O5(g)	0.00E+00	1.75E-28	2.03E-27	5.09E-26	5.81E-25	2.41E-24	4.16E-22	1.65E-22
N2O(g)	0.00E+00	2.18E-11	6.19E-11	2.46E-10	6.96E-10	1.28E-09	1.16E-08	7.80E-09
HNO(g)	0.00E+00	1.13E-12	1.90E-12	3.72E-12	6.09E-12	8.03E-12	1.55E-11	1.52E-11
HNO2(g)	0.00E+00	3.00E-10	7.15E-10	2.23E-09	5.16E-09	8.34E-09	3.36E-08	2.89E-08

Ar(g)	0.00E+00	1.00E-04	2.00E-04	5.00E-04	1.00E-03	1.50E-03	6.50E-03	5.00E-03
BrBrO(g)	4.38E-21	1.05E-18	1.97E-18	4.35E-18	7.43E-18	9.79E-18	9.34E-18	1.28E-17
BrF(g)	9.89E-15	1.52E-13	2.08E-13	3.04E-13	3.86E-13	4.31E-13	2.71E-13	3.78E-13
BrOBr(g)	9.20E-20	2.20E-17	4.14E-17	9.14E-17	1.56E-16	2.06E-16	1.96E-16	2.68E-16
BrOO(g)	6.85E-17	7.98E-14	1.85E-13	5.50E-13	1.21E-12	1.89E-12	5.57E-12	5.33E-12
CH3(g)	4.53E-27	1.84E-31	5.26E-32	9.68E-33	2.50E-33	1.06E-33	8.87E-36	3.43E-35
Cl2O(g)	1.45E-17	4.57E-15	9.14E-15	2.22E-14	4.22E-14	5.98E-14	1.07E-13	1.17E-13
ClClO(g)	0.00E+00	1.39E-14	2.77E-14	6.74E-14	1.28E-13	1.82E-13	3.25E-13	3.56E-13
ClF(g)	2.30E-14	4.05E-13	5.71E-13	8.77E-13	1.18E-12	1.36E-12	1.17E-12	1.46E-12
ClO2(g)	3.34E-17	4.47E-14	1.07E-13	3.33E-13	7.74E-13	1.25E-12	5.06E-12	4.33E-12
ClOCl(g)	4.38E-17	1.38E-14	2.76E-14	6.70E-14	1.27E-13	1.81E-13	3.24E-13	3.54E-13
ClOO(g)	3.30E-16	4.41E-13	1.06E-12	3.29E-12	7.65E-12	1.24E-11	5.00E-11	4.28E-11
COCl(g)	1.46E-14	3.40E-15	2.81E-15	2.13E-15	1.65E-15	1.37E-15	2.53E-16	4.58E-16
COCl2(g)	8.15E-17	7.98E-17	7.85E-17	7.34E-17	6.58E-17	5.88E-17	1.01E-17	2.04E-17
COOH(g)	1.91E-13	4.45E-14	3.68E-14	2.79E-14	2.16E-14	1.80E-14	3.32E-15	6.02E-15
COS(g)	1.40E-14	2.40E-18	8.17E-19	1.92E-19	5.99E-20	2.91E-20	5.31E-22	1.61E-21
CS(g)	6.48E-25	6.24E-30	1.50E-30	2.21E-31	4.88E-32	1.93E-32	1.69E-34	5.86E-34
CS2(g)	1.04E-27	3.10E-35	3.62E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36
H2S(g)	5.56E-12	9.56E-16	3.25E-16	7.63E-17	2.38E-17	1.15E-17	2.08E-19	6.37E-19
H2S2(g)	3.71E-21	1.97E-27	3.28E-28	2.95E-29	4.31E-30	1.31E-30	2.16E-33	1.24E-32
HClCO(g)	7.97E-17	4.38E-18	3.03E-18	1.79E-18	1.13E-18	8.26E-19	6.77E-20	1.57E-19
HCN(g)	0.00E+00	1.72E-23	9.98E-24	4.75E-24	2.59E-24	1.76E-24	1.55E-25	3.21E-25
HCO(g)	2.03E-17	2.65E-19	1.55E-19	7.38E-20	4.04E-20	2.74E-20	2.42E-21	5.01E-21
HCOOH(g)	9.24E-13	5.07E-14	3.50E-14	2.08E-14	1.32E-14	9.59E-15	7.87E-16	1.82E-15
HIO(g)	2.15E-09	9.10E-09	1.07E-08	1.28E-08	1.39E-08	1.41E-08	5.43E-09	8.63E-09
HNCO(g)	0.00E+00	1.15E-18	9.47E-19	7.15E-19	5.53E-19	4.59E-19	8.46E-20	1.54E-19
HS(g)	5.29E-13	3.86E-16	1.57E-16	4.72E-17	1.80E-17	9.94E-18	4.04E-19	9.69E-19
HSO3Cl(g)	3.23E-12	5.61E-11	7.77E-11	1.15E-10	1.45E-10	1.59E-10	5.44E-11	9.78E-11
HSO3F(g)	2.30E-12	3.99E-11	5.54E-11	8.24E-11	1.04E-10	1.13E-10	3.89E-11	7.00E-11
IBr(g)	0.00E+00	1.36E-10	1.55E-10	1.76E-10	1.82E-10	1.78E-10	4.99E-11	8.86E-11
ICl(g)	1.74E-09	7.34E-09	8.61E-09	1.03E-08	1.12E-08	1.14E-08	4.37E-09	6.94E-09
IF(g)	3.13E-13	1.32E-12	1.55E-12	1.86E-12	2.03E-12	2.06E-12	7.92E-13	1.26E-12
IOO(g)	3.56E-17	1.14E-14	2.27E-14	5.52E-14	1.04E-13	1.48E-13	2.68E-13	2.91E-13
N(g)	0.00E+00	5.80E-18	8.20E-18	1.30E-17	1.83E-17	2.25E-17	4.68E-17	4.10E-17
N2O2(g)	0.00E+00	1.36E-18	5.51E-18	3.47E-17	1.39E-16	3.14E-16	5.93E-15	3.50E-15
N2O3(g)	0.00E+00	4.72E-20	2.71E-19	2.70E-18	1.54E-17	4.25E-17	1.68E-15	8.66E-16
NBr(g)	0.00E+00	3.68E-17	5.99E-17	1.12E-16	1.74E-16	2.20E-16	3.10E-16	3.40E-16
NH2(g)	0.00E+00	1.74E-17	1.72E-17	1.66E-17	1.57E-17	1.48E-17	6.05E-18	8.68E-18
NH2OH(g)	0.00E+00	8.53E-19	9.97E-19	1.19E-18	1.31E-18	1.33E-18	5.04E-19	8.09E-19
NH3(g)	0.00E+00	1.40E-14	1.15E-14	8.69E-15	6.72E-15	5.56E-15	1.01E-15	1.85E-15
NO2Cl(g)	0.00E+00	1.64E-15	5.54E-15	2.73E-14	8.97E-14	1.78E-13	1.50E-12	1.12E-12
NOBr(g)	0.00E+00	5.88E-13	1.36E-12	4.02E-12	8.84E-12	1.38E-11	4.05E-11	3.88E-11
NOCl(g)	0.00E+00	5.82E-11	1.39E-10	4.31E-10	9.99E-10	1.61E-09	6.50E-09	5.57E-09
NOF(g)	0.00E+00	1.18E-14	2.80E-14	8.73E-14	2.02E-13	3.27E-13	1.32E-12	1.13E-12
NOI(g)	0.00E+00	1.34E-14	2.67E-14	6.46E-14	1.22E-13	1.73E-13	3.11E-13	3.39E-13

NS(g)	0.00E+00	1.82E-19	1.26E-19	7.64E-20	5.05E-20	3.88E-20	7.39E-21	1.22E-20
OBrO(g)	1.33E-19	1.55E-16	3.60E-16	1.07E-15	2.35E-15	3.67E-15	1.08E-14	1.04E-14
OIO(g)	1.05E-19	3.37E-17	6.71E-17	1.63E-16	3.09E-16	4.37E-16	7.92E-16	8.62E-16
S(g)	3.84E-14	1.19E-16	5.80E-17	2.23E-17	1.04E-17	6.54E-18	5.98E-19	1.12E-18
S2(g)	4.46E-16	4.27E-21	1.02E-21	1.50E-22	3.28E-23	1.29E-23	1.08E-25	3.82E-25
S2Br2(g)	2.58E-27	3.32E-31	1.04E-31	2.15E-32	5.64E-33	2.39E-33	9.15E-36	5.04E-35
S2Cl(g)	2.64E-20	1.07E-24	3.01E-25	5.50E-26	1.39E-26	5.89E-27	4.57E-29	1.80E-28
S2Cl2(g)	5.62E-24	9.52E-28	3.19E-28	7.21E-29	2.11E-29	9.63E-30	6.92E-32	3.05E-31
S2O(g)	5.38E-15	9.19E-19	3.11E-19	7.28E-20	2.25E-20	1.09E-20	1.90E-22	5.88E-22
S3(g)	3.22E-25	9.57E-33	1.11E-33	6.30E-35	6.43E-36	1.59E-36	1.00E-36	1.00E-36
S4(g)	2.89E-34	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36
S5(g)	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36
S6(g)	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36
SBr2(g)	2.54E-17	1.06E-18	6.82E-19	3.65E-19	2.05E-19	1.39E-19	5.79E-21	1.70E-20
SCl(g)	2.57E-15	3.34E-17	1.93E-17	9.20E-18	4.98E-18	3.36E-18	2.85E-19	5.98E-19
SCl2(g)	1.44E-15	7.88E-17	5.41E-17	3.19E-17	2.00E-17	1.45E-17	1.14E-18	2.67E-18
SF(g)	7.85E-18	1.02E-19	5.91E-20	2.82E-20	1.52E-20	1.03E-20	8.74E-22	1.84E-21
SO(g)	2.72E-08	1.50E-09	1.04E-09	6.34E-10	4.20E-10	3.23E-10	6.18E-11	1.02E-10
SO2Cl2(g)	5.82E-16	1.01E-14	1.40E-14	2.08E-14	2.61E-14	2.85E-14	9.78E-15	1.76E-14
SO2ClF(g)	5.95E-16	1.03E-14	1.43E-14	2.13E-14	2.68E-14	2.92E-14	1.01E-14	1.81E-14
SO3(g)	5.66E-06	9.94E-05	1.39E-04	2.13E-04	2.83E-04	3.28E-04	2.74E-04	3.45E-04
SOCl(g)	7.07E-11	1.64E-11	1.35E-11	1.02E-11	7.80E-12	6.46E-12	1.14E-12	2.10E-12
SOCl2(g)	4.44E-14	4.33E-14	4.23E-14	3.95E-14	3.50E-14	3.12E-14	5.12E-15	1.05E-14
SOF(g)	4.70E-11	1.09E-11	8.96E-12	6.78E-12	5.19E-12	4.30E-12	7.63E-13	1.40E-12

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