Institute	Model	
Univ. Bremen, Inst. Umweltph.	BRAPHO	(Box)
FZ Jülich, Inst. Strat. Chemie	CLaMS	(Box)
	FACSIMILE	(Box)
FZ Karlsruhe, Inst. Met. + Klima	KASIMA	(Box,3-D)
Univ. Köln, Geophysik	COMMA	(Box,3-D)
Univ. Köln, Geophysik	EURAD–TS	(Box,3-D)
MPI Mainz, Luftchemie	FACSIMILE	(Box)
MPI Mainz, Luftchemie	MPIC	(Box,2-D)
AWI Potsdam	AWIP	(Box)

Table 1: List of models participating in the OFP model intercomparison.

Model	Photolysis	Chemistry	
		GAS PHASE	HETEROGENEOUS
BRAPHO	PHOTOGT [P1]	gear, ASAD–2[G1], reaction list + rates	Carslaw–Het6[H1,H2]
CLaMS	Lary [P2]	family, ASAD–2[G1], reaction list + rates	Carslaw–Het6[H3]
KASIMA	R¨oth[P3]	family, iterative Euler backward[G2]	PSC–formation after H+M[H1] + Carslaw–Het6[H2]
COMMA	Brasseur[P4]	family, reaction systems[G3]	PSC–formation after H+M[H1,H4,H5]
EURAD–TS	Madronich[P5]	family, semi–implicit, QSSA, reaction list + rates	no het. chem. implemented
FACSIMILE	Lary [P2]	gear, reaction list + rates	Carslaw–Het6[H2]
MPIC[M1]	Br¨uhl[P6]	family[G4]	PSC–formation after H+M[H1]
AWIP	Brasseur[P7]	family, iterative Euler backward	PSC–formation after H+M[H1] + Carslaw–Het6[H2]

Table 2: Description of the models.

The calculations of all participating models were performed in the box model mode; all models use rate constants compiled by DeMore et al. (1997).

P1: Blindauer et al. (1996); **P2:** Lary and Pyle (1991), Becker et al. (2000a); **P3:** $j = a \cdot \exp\left(b \cdot \left(1 - \frac{1}{\cos(c \cdot \chi)}\right)\right)$, a, b, c from tables ($\Rightarrow$ standard photolysis for model intercomparison; R¨oth, 1992); **P4:** Brasseur et al. (1990), Granier and Brasseur (1992) + updates. **P5:** Madronich (1987); **P6:** Zdunkowski (1980), Br¨uhl and Crutzen (1989); **P7:** Brasseur et al. (1997); photolysis rates from precalculated tables, calculation of optical thickness with Chapman function;

G1: Carver et al (1997); **G2:** Ruhnke et al. (1999); **G3:** based on Kr¨uger and Fabian (1986); **G4:** Crutzen and Schmailzl (1983);

H1: Hanson and Mauersberger (1988); **H2:** Carslaw et al. (1995); **H3:** Carslaw et al. (1997); **H4:** G¨unther et al. (1995); **H5:** sulfate aerosol chemistry as in Hendricks et al. (1999).

M1: The chemistry module of the MPIC model is designed to calculate average values for a zonal ring at a given latitude and altitude. Therefore, approximations are included to account for the non-linearity of some processes, e.g. a temperature-weighted average of heterogeneous reaction rates using statistics for temperature deviation from zonal mean. Here, these temperature-weighted average is not used, however, the shown results suffer from assumptions made in this module as the neglect of the thermal decomposition of Cl_2O_2. This may lead to inaccurate results if this routine is used in a box model mode. Thus, the MPIC results are not fully comparable with the other participating models.

	ARCTIC 1995					ANTARCTIC 1995	
Scenario group	unprescribed	prescribed					
		trajec. 1		trajec. 2		trajec. 1	trajec. 2
Trajectory time	94, Dec.15 – Feb.3	Jan.11 –	Feb.10	Feb.10 –	Mar.31	Jul.30 – Sep.13	Sep.13 – Oct.31
Scenario type	CASE STUDY	GPH[a]	GPH + HET[b]	GPH	GPH + HET	GPH + HET	GPH + HET
Levels (K)	435, 475, 500, 550 600, 675	420 475 600	475	420 475 600	475	475	475
Init. Gas Phase[e]	Woyke et al. (1999)	2D–Model[f]		$t_{end}^{1(GPh)}$[g]	$t_{end}^{1(GPh+Het)}$[h]	2D–Model[f]	$t_{end}^{1(GPh+Het)}$[i]
Init. liq. aerosol[d]	Woyke et al. (1999)	standardized H_2SO_4, σ, S_{liq}, S_{ice}					
PSC microphys.[d]	individual	standardized N_{liq}, N_{NAT}, N_{ice}, $Supersat_{NAT}$, $Supersat_{ice}$					
Photolysis	individual	standardized after Röth, 1992[c]					

Table 3: Overview of the scenarios of the model intercomparison; for more information see text; for scenario acronyms see Table 4.

[a] GPH: model runs include only gas phase chemistry;

[b] GPH + HET: model runs including both gas phase + heterogeneous chemistry;

[c] $j = a \cdot \exp\left(b \cdot \left(1 - \frac{1}{\cos(c \cdot \chi)}\right)\right)$, a, b, c from tables for 115 reactions, $j = 0$ for $\chi > 100°$ and $(c \cdot \chi) > 90°$, j: photolysis rates, χ: solar zenith angle (SZA);

[d] Detailed standardizations and initializations see Table 5;

[e] Detailed initializations see Table 6;

[f] Initial values determined by MPIC–2D–Model (Gidel et al., 1983; Grooß, 1996);
for the GPH run the complete activation of chlorine and bromine is included in the initialization.

[g] Initial values taken from ARCTIC 1 (GPH) at t_{end}.

[h] Initial values taken from ARCTIC 1 (GPH+HET) at t_{end}.

[i] Initial values taken from ANTARCTIC 1 (GPH+HET) at t_{end} but corrected for dehydration and denitrification.

SCENARIO ACRONYM				scenario type	scenario group
ARCTIC 1 (GPH[a]):	Arctic 1995	475 K	trajectory 1	only gas phase	prescribed
ARCTIC 1 (GPH + HET[b]):	Arctic 1995	475 K	trajectory 1	gas phase + heterog.	prescribed
ARCTIC 1 (GPH)$^{\text{ind. photol. rate}}$:	same as ARCTIC 1 (GPH), but with individual photolysis rates				
ARCTIC 2 (GPH):	Arctic 1995	475 K	trajectory 2	only gas phase	prescribed
ARCTIC 2 (GPH + HET):	Arctic 1995	475 K	trajectory 2	gas phase + heterog.	prescribed
ANTARCTIC 1 (GPH + HET):	Antarctic 1995	475 K	trajectory 1	gas phase + heterog.	prescribed
ANTARCTIC 2 (GPH + HET):	Antarctic 1995	475 K	trajectory 2	gas phase + heterog.	prescribed
ARCTIC CASE STUDY:	Arctic 1995	6 levels and trajectories		gas phase + heterog.	unprescribed

Table 4: Acronyms for the different scenarios (used throughout the text; for detailed description of the scenarois see text and Table 3)

[a] GPH: model runs include only gas phase chemistry;

[b] GPH + HET: model runs including both gas phase + heterogeneous chemistry.

		ARCTIC 1 GPH + HET	ARCTIC 2 GPH + HET	ANTARCTIC 1 GPH + HET	ANTARCTIC 2 GPH + HET
				Initialization of STS aerosol	
H_2SO_4	ppb	0.5	0.5	0.2	0.2
σ		1.8	1.8	1.8	1.8
T(t=0)	K	197.0	205.4	182.4	200.2
p(t=0)	hPa	46.0	53.5	35.3	48.6
N_{STS}	$\frac{1}{cm^3}$	10.0	10.0	12.5	15.7
S_{STS}	$\frac{\mu m^2}{cm^3}$	2.09	2.02	1.31	1.21
				Standardized PSC settings	
$Supersat_{NAT,ice}$		1	1	1	1
N_{NAT}	$\frac{1}{cm^3}$	1.0	1.0	1.0	1.0
N_{ice}	$\frac{1}{cm^3}$			0.01	
S^a_{ice}	$\frac{\mu m^2}{cm^3}$			22.2	

Table 5: Initialization of STS (supercooled liquid ternary solution) background aerosol particles and settings for PSC (polar stratospheric cloud) microphysics for the prescribed scenarios.

The number density distribution of the initial STS aerosol particles is lognormal with a given width σ and the particles are formed from H_2SO_4; $S_{STS,NAT,ice}$: total surface density of STS, NAT or ice particles; $N_{STS,NAT,ice}$: number density of STS, NAT or ice particles; $Supersat_{NAT,ice}$: supersaturation for NAT or ice formation; T: temperature, p: pressure.

[a] Because ice is already present at the beginning of the ANTARCTIC 1 (GPH + HET) scenario, S_{ice} is initialized here; for a definition of scenarios see Tables 3 and 4; for more information see text.

	ARCTIC 1		ARCTIC 2		ANTARCTIC 1	ANTARCTIC 2
	GPH[a]	GPH + HET	GPH	GPH + HET	GPH + HET	GPH[b] + HET
				ppmv		
O_3	4.91		4.53		5.00	2.95
H_2O	3.67		3.67		4.50	1.89
N_2O	0.10		0.10		0.13	0.13
CH_4	1.01		1.00		0.96	0.96
H_2	0.55		0.56		0.53	0.50
				ppbv		
HNO_3	15.04	13.42	14.11		9.00	2.50
$ClONO_2$	0.0	0.76	1.59		1.20	0.11
HCl	0.0	1.14	0.24		1.80	0.13
ClO	1.91	$1.97 \cdot 10^{-3}$	2.59		$3.96 \cdot 10^{-2}$	0.73
Cl_2O_2	$3.42 \cdot 10^{-2}$		$5.95 \cdot 10^{-3}$		0.0	0.87
N_2O_5	0.0	0.81	$7.97 \cdot 10^{-3}$		$6.65 \cdot 10^{-3}$	$1.99 \cdot 10^{-6}$
CO	20.08		23.92		16.97	16.34
NO_2	0.31		0.056		1.89	$0.23 \cdot 10^{-3}$
HNO_4	0.409		0.096		0.10	$4.98 \cdot 10^{-4}$
				pptv		
BrO	17.18	$2.43 \cdot 10^{-3}$	0.13		7.27	6.69
$BrONO_2$	0.0		8.51		0.0	$7.70 \cdot 10^{-4}$
BrCl	0.0		1.51		0.0	8.28
HBr	0.0	2.18	1.39		8.51	$4.85 \cdot 10^{-4}$
Br	0.0	7.50	3.89		0.0	0.13
HOBr	0.0	7.50	5.65		0.0	0.50
H_2O_2	12.38		25.0		6.36	0.40
CH_2O	8.78		95.6		24.5	12.42
Cl_2	0.0		0.12		0.0	$9.34 \cdot 10^{-4}$
HOCl	3.98		94.6		5.46	116.00
OClO	0.0		10.4		0.0	15.20
NO_3	0.0		2.98		0.0	$1.08 \cdot 10^{-4}$

Table 6: Initializations of gas phase chemistry for the prescribed scenarios.

[a] activated gas phase chemistry [HCl + $ClONO_2 \Rightarrow$ ClO, HBr + Br + HOBr $\Rightarrow$ BrO, $N_2O_5 \Rightarrow 2 \cdot HNO_3$];

[b] artificial denitrification [$(NO_y)^{\text{Antarctic2}}_{t=0} = \frac{1}{4}(NO_y)^{\text{Antarctic1}}$] and dehydration [$(H_2O)^{\text{Antarctic2}}_{t=0} = \min(H_2O)^{\text{Antarctic1}}$], for details see text.

For definition of scenarios see Tables 3 and 4.

		ARCTIC 1		ARCTIC 2		ANTARCTIC 1	ANTARCTIC 2
CASE STUDY		GPH	GPH + HET	GPH	GPH + HET	GPH + HET	GPH + HET
Scenario group	unprescribed	prescribed					
Init. O_3, ppm	3.21	4.91	4.91	4.57	4.52	5.00	3.03
Mean End O_3, ppm	2.49	4.57	4.52	4.39	4.25	3.03	0.66
Mean O_3 – loss, ppm	0.72	0.34	0.39	0.18	0.27	1.97	2.37
STD–deviation, ppm	±0.21	±0.02	±0.11	±0.01	±0.02	±0.13	±0.10
Mean O_3 – loss, abs. %	22.3	7.0	7.9	3.9	6.0	39.4	78.2
STD–deviation, abs. %	±6.7	±0.3	±1.2	±0.2	±0.4	±2.5	±3.3
		5.1 ±1.0 ARCTIC 1 (GPH)$^{\text{ind. photol. rate}}$					

Table 7: Mean overall ozone loss in the different scenarios and scatter of model results around the mean value. For definition of scenarios see Tables 3 and 4.

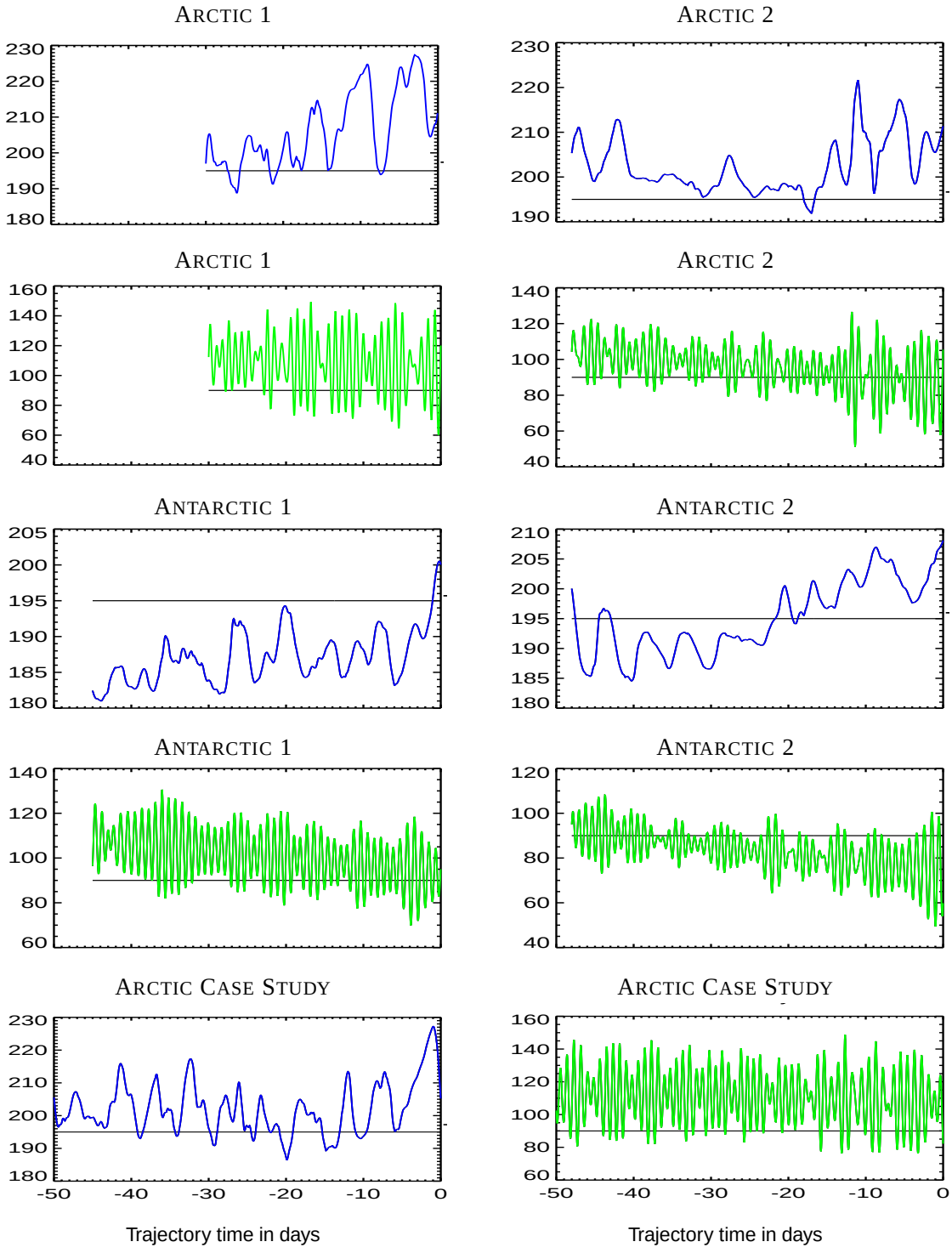

Figure 1: Scenario trajectories (potential temerature 475K, timestep one hour):
Temperature (K, 195K is indicated) and Solar Zenith Angle (deg, 90° is indicated).

ARCTIC 1 + 2:	11.1.	–	10.2.	–	31.03. 1995
ANTARCTIC 1 + 2:	30.7.	–	13.9.	–	31.10. 1995
ARCTIC CASE STUDY:	15.12.1994			–	3.2. 1995

For definition of scenarios see Tables 3 and 4.

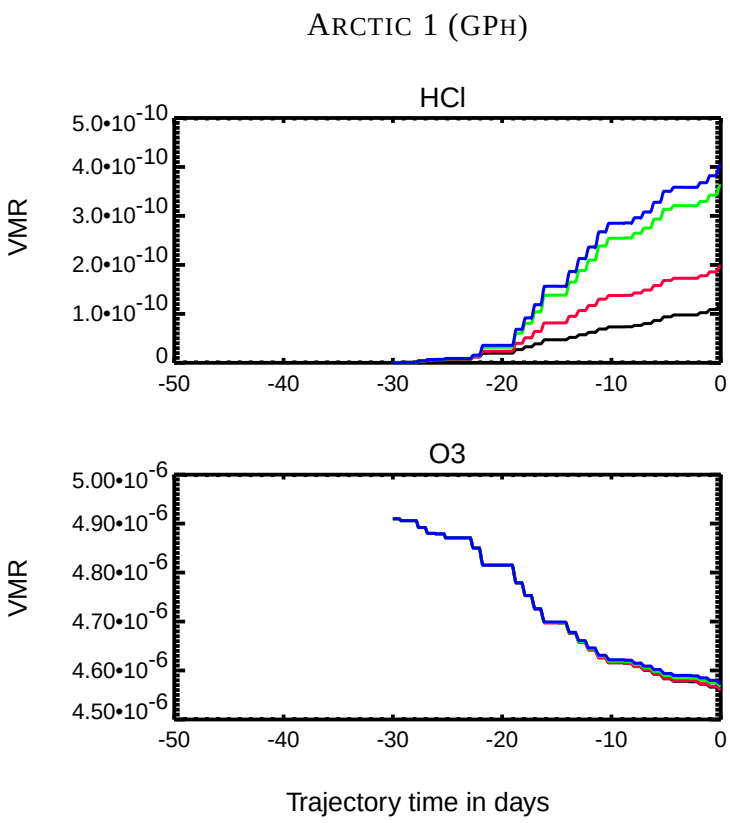

Figure 2: Volume mixing ratios versus trajectory time for the scenario ARCTIC 1 (GPH): Development of HCl and O_3 when enabling the four known major source reactions for HCl in the stratosphere one after another using the KASIMA model.

black: s1, **red: s1 + s2**, **green: s1 + s2 + s3**, **blue: s1 + s2 + s3 + s4**

(r1) $Cl + CH_4 \longrightarrow HCl + CH_3$

(r2) $ClO + OH \xrightarrow{\sim 6\%} HCl + O_2$ (Lipson et al., 1997)

(r3) $ClO + HO_2 \xrightarrow{\sim 3\%} HCl + O_3$ (Finkbeiner et al., 1995)

(r4) $HOCl + h\nu \xrightarrow{\sim 2\%} HCl + O$ (possible contribution after DeMore et al., 1997)

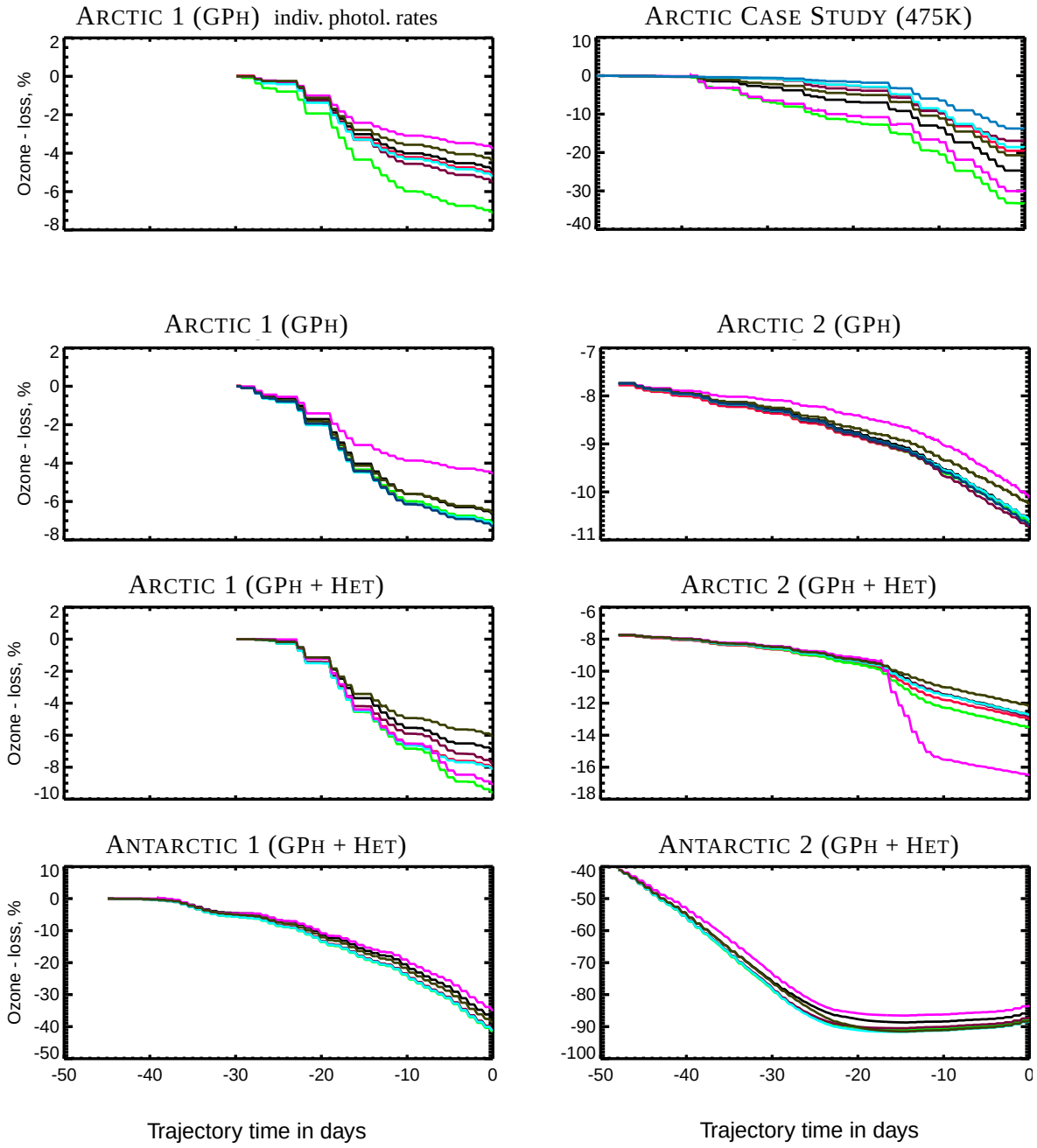

Figure 3: Percentage ozone loss calculated by all participating models for all considered scenarios at 475K.

ARCTIC 1 + 2:	11.1.	–	10.2.	–	31.03. 1995 (prescr. boundary cond.)
ANTARCTIC 1 + 2:	30.7.	–	13.9.	–	31.10. 1995 (prescribed)
ARCTIC CASE STUDY:	15.12.1994			–	3.2. 1995 (unprescribed)

Reference point for the 2th scenarios are the initial values of the respective 1th scenario; for definition of models see Tables 1 and 2, scenarios see Tables 3 and 4.

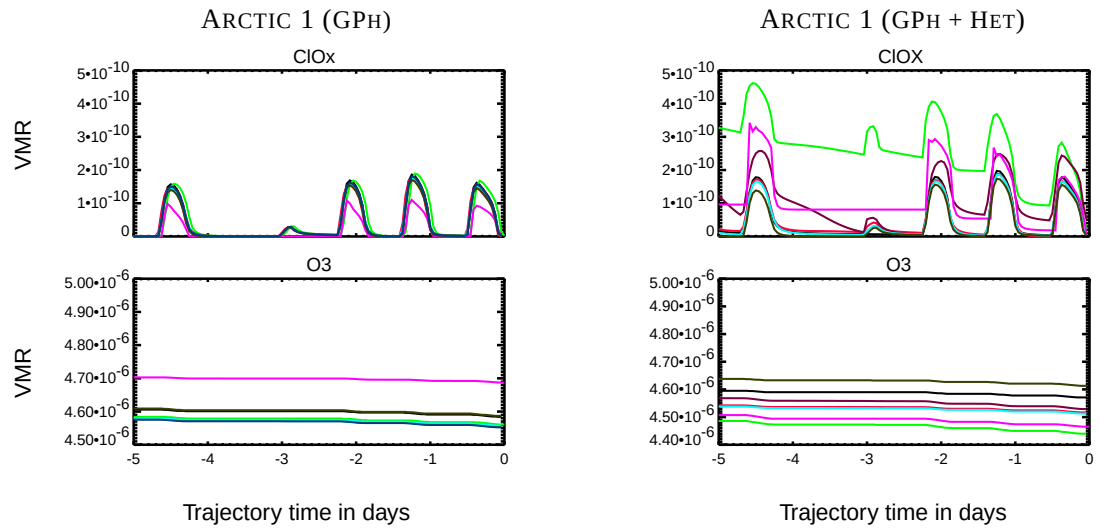

Figure 4: Volume mixing ratios of ClO_x and O_3 versus trajectory time for the last five days of the scenarios ARCTIC 1 (GPH) and (GPH + HET).

For definition of models see Tables 1 and 2, scenarios see Tables 3 and 4.

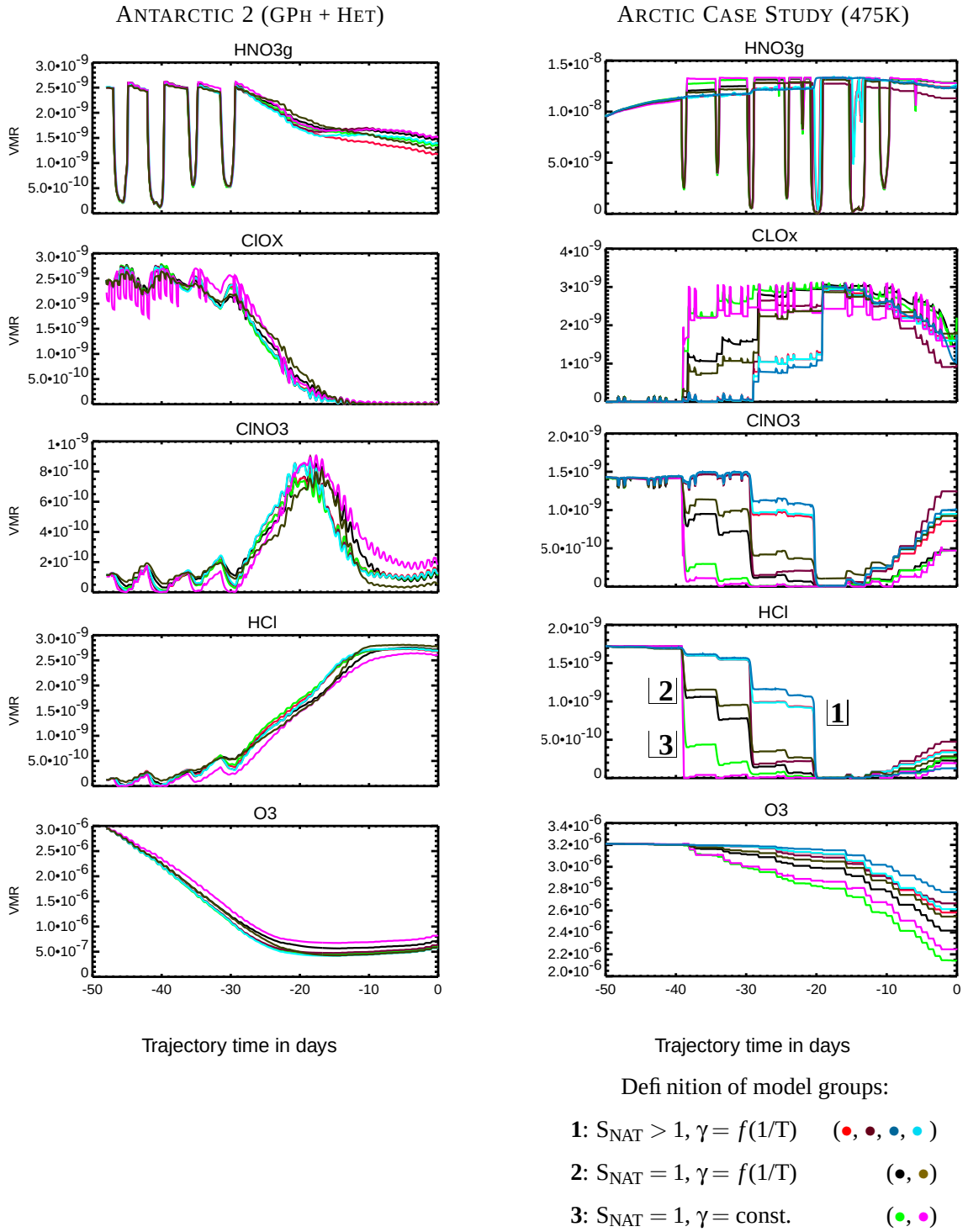

Figure 5: Examples for the agreement of models (gaseous components):

volume mixing ratios of various gaseous components along two 475K trajectories; left panel (ANTARCTIC 2, 13.9. – 31.10. 1995): under prescribed conditions (standardized PSC microphysics and photolysis rates); right panel (ARCTIC CASE STUDY, 15.12. 1994 – 3.2. 1995): under unprescribed conditions; for definition of models see Tables 1 and 2, scenarios see Tables 3 and 4.

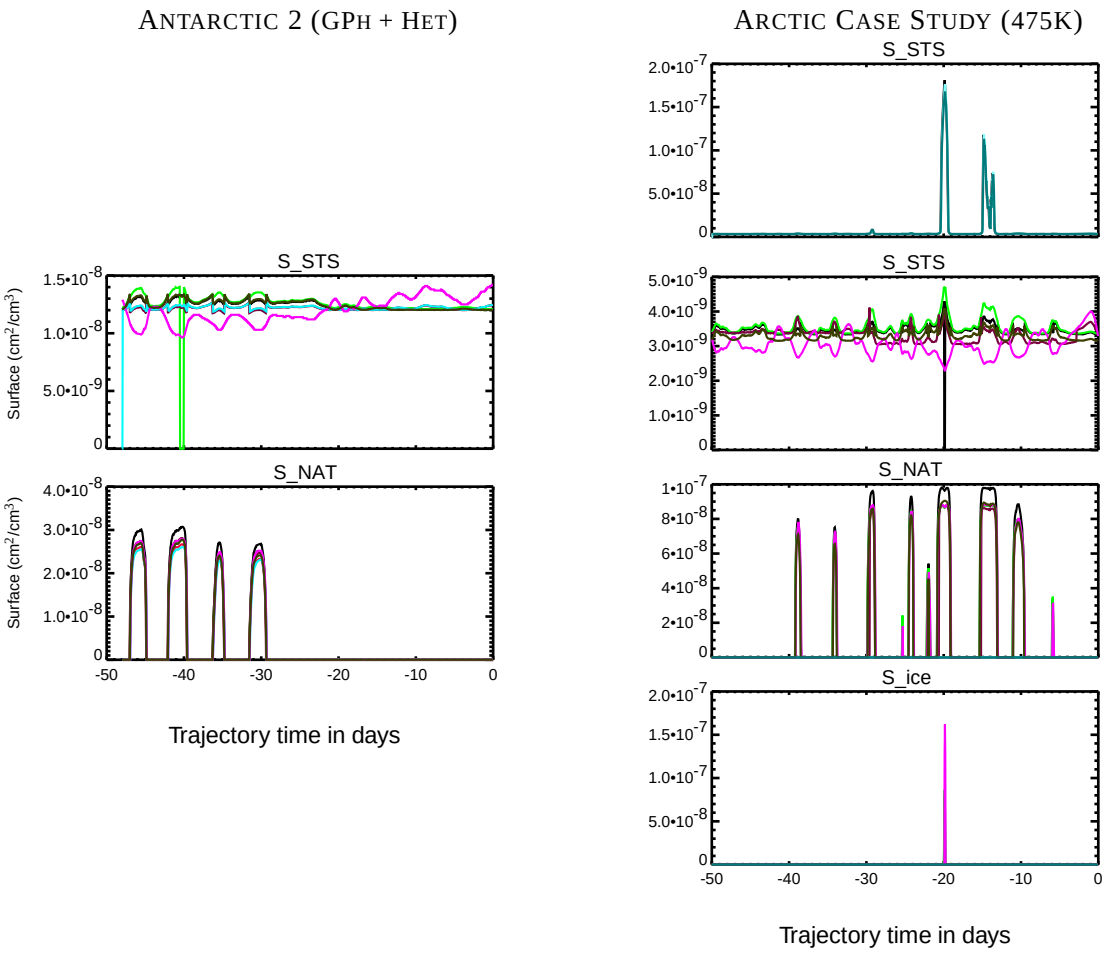

Figure 6: Same as Figure 5, but heterogeneous reaction surfaces.

In the right panel the upper two figures show S_{STS} but with different scales: the upper figure shows those models using strongly supercooled conditions for NAT formations with the effect that the gaseous nitric acid agglomerates on the STS aerosols.

For definition of models see Tables 1 and 2, scenarios see Tables 3 and 4.

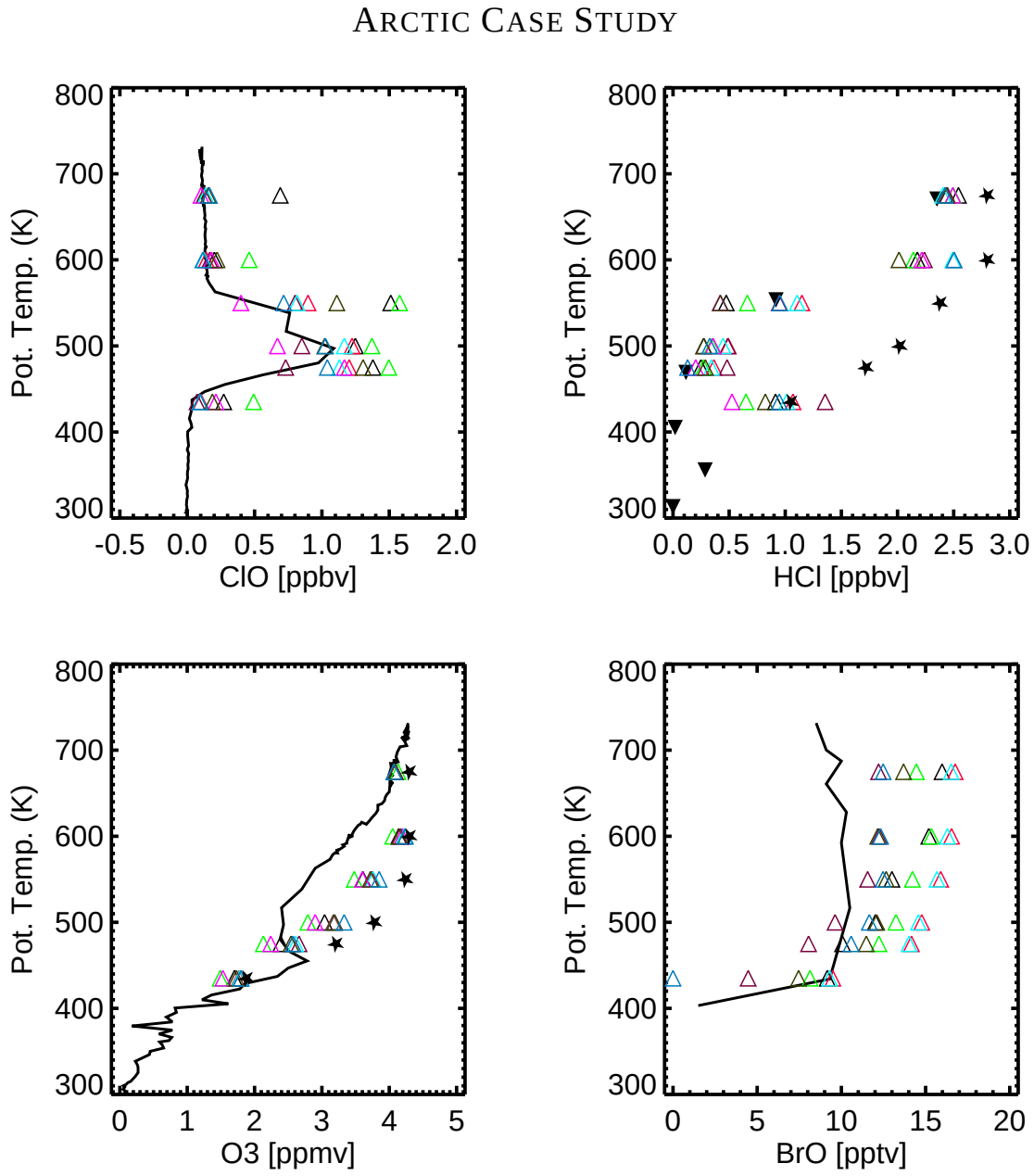

Figure 7: Comparison of measurements with model calculations in the unprescribed ARCTIC CASE STUDY.

Solid lines: Balloon–based profiles of O_3, ClO and BrO, measured in Kiruna, Sweden, on Feb. 3, 1995*; **black triangles**: HCl profile, derived from HALOE observations on Jan. 26 – 28 and Feb. 6 – 7*; **stars**: initial values on Dec. 15, 1994*; **colored triangles**: end values (Feb. 3, 1995) of model calculations along the six trajectories of the ARCTIC CASE STUDY;

* from Pierson et al. (1999) and Woyke et al. (1999);

for definition of models see Tables 1 and 2, scenarios see Tables 3 and 4.