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Mountain-wave-induced polar stratospheric clouds and their representation in the global chemistry model ICON-ART

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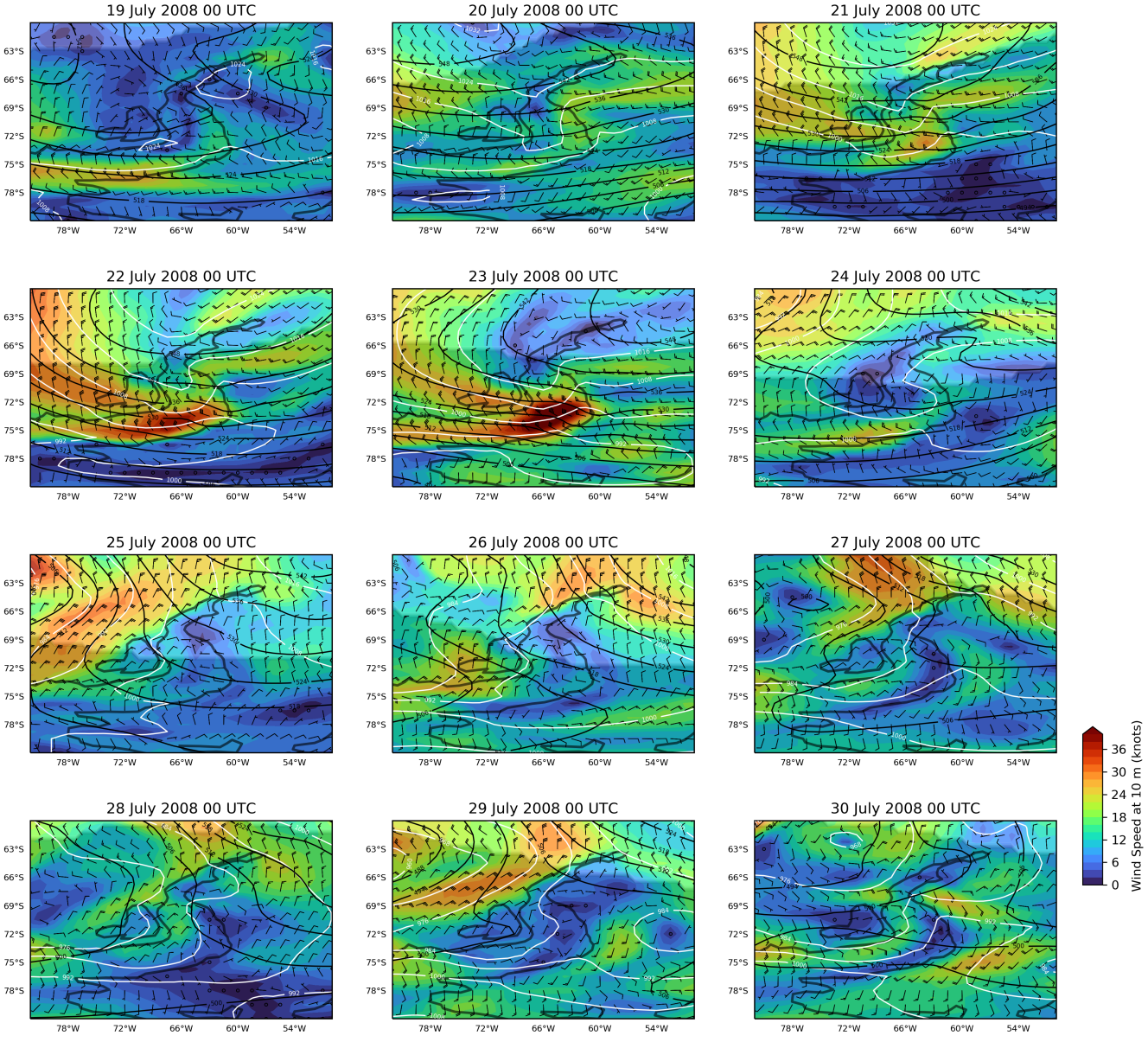

Figure S1. Fig. 4 of the main paper, but for every day between 19 and 30 July 2008.

Table S1. Gasphase reactions. The reaction rates constants in the second column are given in units of either cm^3s^{-1} or cm^6s^{-2} depending on the type of the reaction. Reaction rate constants are provided by the MECCA module, incorporated in ICON-ART. Terms in the reaction rate constants are: `cair` and `cH2O` concentrations of air and H_2O in cm^{-3} and `temp` air temperature in K. `k_3rd` refers to equations for threr body reactions by Jet Propulsion Laboratory (Sander et al., 2011). The abbreviated reaction rate constants are shown in the respective reaction directly above.

Reaction	Rate Constant (cgs-system)
$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	`3.3E-11*EXP(55./temp)`
$O_2 + O(^3P) + M \rightarrow O_3 + M$	`6.E-34*((temp/300.)**(-2.4))*cair`
$O_3 + O(^1D) \rightarrow 2\ O_2$	`1.2E-10`
$O_3 + O(^3P) \rightarrow 2\ O_2$	`8.E-12*EXP(-2060./temp)`
$H + O_2 + M \rightarrow HO_2 + M$	`k_3rd(temp,cair,4.4E-32,1.3,7.5E-11,-0.2,0.6)`
$H + O_3 \rightarrow OH + O_2$	`1.4E-10*EXP(-470./temp)`
$H_2 + O(^1D) \rightarrow H + OH$	`1.2E-10`
$OH + O(^3P) \rightarrow H + O_2$	`1.8E-11*EXP(180./temp)`
$OH + O_3 \rightarrow HO_2 + O_2$	`1.7E-12*EXP(-940./temp)`
$OH + H_2 \rightarrow H_2O + H$	`2.8E-12*EXP(-1800./temp)`
$HO_2 + O(^3P) \rightarrow OH + O_2$	`3.E-11*EXP(200./temp)`
$HO_2 + O_3 \rightarrow OH + 2\ O_2$	`1.E-14*EXP(-490./temp)`
$HO_2 + H \rightarrow 2\ OH$	`7.2E-11`
$HO_2 + H \rightarrow H_2 + O_2$	`6.9E-12`
$HO_2 + H \rightarrow O(^3P) + H_2O$	`1.6E-12`
$HO_2 + OH \rightarrow H_2O + O_2$	`4.8E-11*EXP(250./temp)`
$HO_2 + HO_2 + M \rightarrow H_2O_2 + O_2 + M$	`(1.5E-12*EXP(19./temp)+1.7E-33*EXP(1000./temp)*cair)* (1.+1.4E-21*EXP(2200./temp)*cH2O)`
$H_2O + O(^1D) \rightarrow 2\ OH$	`1.63E-10*EXP(60./temp)`
$H_2O_2 + OH \rightarrow H_2O + HO_2$	`1.8E-12`
$N + O_2 \rightarrow NO + O(^3P)$	`1.5E-11*EXP(-3600./temp)`
$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	`2.15E-11*EXP(110./temp)`
$N_2O + O(^1D) \rightarrow 2\ NO$	`7.25E-11*EXP(20./temp)`
$N_2O + O(^1D) \rightarrow N_2 + O_2$	`4.63E-11*EXP(20./temp)`
$NO + O_3 \rightarrow NO_2 + O_2$	`3.E-12*EXP(-1500./temp)`
$NO + N \rightarrow O(^3P) + N_2$	`2.1E-11*EXP(100./temp)`
$NO_2 + O(^3P) \rightarrow NO + O_2$	`5.1E-12*EXP(210./temp)`
$NO_2 + O_3 \rightarrow NO_3 + O_2$	`1.2E-13*EXP(-2450./temp)`
$NO_2 + N \rightarrow N_2O + O(^3P)$	`5.8E-12*EXP(220./temp)`
$NO_3 + NO \rightarrow 2\ NO_2$	`1.5E-11*EXP(170./temp)`
$NO_3 + NO_2 + M \rightarrow N_2O_5 + M$	`k_3rd(temp,cair,2.0E-30,4.4,1.4E-12,0.7,0.6)`
$N_2O_5 + M \rightarrow NO_2 + NO_3 + M$	`k_NO3_NO2/(2.7E-27*EXP(11000./temp))`
$NO + HO_2 \rightarrow NO_2 + OH$	`3.3E-12*EXP(270./temp)`
$NO_2 + OH + M \rightarrow HNO_3 + M$	`k_3rd(temp,cair,1.8E-30,3.0,2.8E-11,0.,0.6)`
$NO_2 + HO_2 + M \rightarrow HNO_4 + M$	`k_3rd(temp,cair,2.0E-31,3.4,2.9E-12,1.1,0.6)`
$HNO_3 + OH \rightarrow H_2O + NO_3$	`2.4E-14*EXP(460./temp) + 1./ ( 1./(6.5E-34* EXP(1335./temp)*cair) + 1./(2.7E-17*EXP(2199./temp)) )`
$HNO_4 + M \rightarrow NO_2 + HO_2 + M$	`k_NO2_HO2/(2.1E-27*EXP(10900./temp))`
$HNO_4 + OH \rightarrow NO_2 + H_2O$	`1.3E-12*EXP(380./temp)`
$CH_4 + O(^1D) \rightarrow .75\ CH_3O_2 + .75\ OH + .25\ HCHO + .4\ H + .05\ H_2$	`1.75E-10`
$CH_4 + OH \rightarrow CH_3O_2 + H_2O$	`1.85E-20*EXP(2.82*log(temp)-987./temp)`
$CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$	`4.1E-13*EXP(750./temp)`
$CH_3O_2 + NO \rightarrow HCHO + NO_2 + HO_2$	`2.8E-12*EXP(300./temp)`
$CH_3O_2 \rightarrow HCHO + HO_2$	`2.*RO2*9.5E-14*EXP(390./temp)/ (1.+1./26.2*EXP(1130./temp))`
$CH_3O_2 \rightarrow .5\ HCHO + .5\ CH_3OH + .5\ O_2$	`2.*RO2*9.5E-14*EXP(390./temp)/(1.+26.2*EXP(-1130./temp))`
$CH_3OOH + OH \rightarrow .7\ CH_3O_2 + .3\ HCHO + .3\ OH + H_2O$	`3.8E-12*EXP(200./temp)`
$HCHO + OH \rightarrow CO + H_2O + HO_2$	`9.52E-18*EXP(2.03*log(temp)+636./temp)`
$CO + OH \rightarrow H + CO_2$	`(1.57E-13+cair*3.54E-33)`

Table S1. Continued.

Reaction	Rate Constant (cgs-system)
$Cl + O_3 \rightarrow ClO + O_2$	2.8E-11*EXP(-250./temp)
$ClO + O(^3P) \rightarrow Cl + O_2$	2.5E-11*EXP(110./temp)
$ClO + ClO \rightarrow Cl_2 + O_2$	1.0E-12*EXP(-1590./temp)
$ClO + ClO \rightarrow 2\ Cl + O_2$	3.0E-11*EXP(-2450./temp)
$ClO + ClO \rightarrow Cl + OClO$	3.5E-13*EXP(-1370./temp)
$ClO + ClO + M \rightarrow Cl_2O_2 + M$	k_3rd_iupac(temp,cair,2.0E-32,4.0,1.0E-11,0.0,0.45)
$Cl_2O_2 + M \rightarrow ClO + ClO + M$	k_ClO_ClO/(1.72E-27*EXP(8649./temp))
$Cl + H_2 \rightarrow HCl + H$	3.9E-11*EXP(-2310./temp)
$Cl + HO_2 \rightarrow HCl + O_2$	4.4E-11-7.5E-11*EXP(-620./temp)
$Cl + HO_2 \rightarrow ClO + OH$	7.5E-11*EXP(-620./temp)
$Cl + H_2O_2 \rightarrow HCl + HO_2$	1.1E-11*EXP(-980./temp)
$ClO + OH \rightarrow .94\ Cl + .94\ HO_2 + .06\ HCl + .06\ O_2$	7.3E-12*EXP(300./temp)
$ClO + HO_2 \rightarrow HOCl + O_2$	2.2E-12*EXP(340./temp)
$HCl + OH \rightarrow Cl + H_2O$	1.7E-12*EXP(-230./temp)
$HOCl + OH \rightarrow ClO + H_2O$	3.0E-12*EXP(-500./temp)
$ClO + NO \rightarrow NO_2 + Cl$	6.2E-12*EXP(295./temp)
$ClO + NO_2 + M \rightarrow ClNO_3 + M$	k_3rd_iupac(temp,cair,1.6E-31,3.4,7.E-11,0.,0.4)
$ClNO_3 + O(^3P) \rightarrow ClO + NO_3$	4.5E-12*EXP(-900./temp)
$ClNO_3 + Cl \rightarrow Cl_2 + NO_3$	6.2E-12*EXP(145./temp)
$Cl + CH_4 \rightarrow HCl + CH_3O_2$	6.6E-12*EXP(-1240./temp)
$Cl + HCHO \rightarrow HCl + CO + HO_2$	8.1E-11*EXP(-34./temp)
$Cl + CH_3OOH \rightarrow HCHO + HCl + OH$	5.9E-11
$ClO + CH_3O_2 \rightarrow HO_2 + Cl + HCHO$	3.3E-12*EXP(-115./temp)
$CCl_4 + O(^1D) \rightarrow ClO + 3\ Cl$	3.3E-10
$CH_3Cl + O(^1D) \rightarrow OH + Cl$	1.65E-10
$CH_3Cl + OH \rightarrow H_2O + Cl$	2.4E-12*EXP(-1250./temp)
$CH_3CCl_3 + O(^1D) \rightarrow OH + 3\ Cl$	3.E-10
$CH_3CCl_3 + OH \rightarrow H_2O + 3\ Cl$	1.64E-12*EXP(-1520./temp)
$CF_2Cl_2 + O(^1D) \rightarrow ClO + Cl$	1.4E-10
$CFCl_3 + O(^1D) \rightarrow ClO + 2\ Cl$	2.3E-10
$Br + O_3 \rightarrow BrO + O_2$	1.7E-11*EXP(-800./temp)
$BrO + O(^3P) \rightarrow Br + O_2$	1.9E-11*EXP(230./temp)
$BrO + BrO \rightarrow 2\ Br + O_2$	2.7E-12
$BrO + BrO \rightarrow Br_2 + O_2$	2.9E-14*EXP(840./temp)
$Br + HO_2 \rightarrow HBr + O_2$	7.7E-12*EXP(-450./temp)
$BrO + HO_2 \rightarrow HOBr + O_2$	4.5E-12*EXP(500./temp)
$HBr + OH \rightarrow Br + H_2O$	6.7E-12*EXP(155./temp)
$HOBr + O(^3P) \rightarrow OH + BrO$	1.2E-10*EXP(-430./temp)
$Br_2 + OH \rightarrow HOBr + Br$	2.0E-11*EXP(240./temp)
$BrO + NO \rightarrow Br + NO_2$	8.7E-12*EXP(260./temp)
$BrO + NO_2 + M \rightarrow BrNO_3 + M$	k_3rd_iupac(temp,cair,4.7E-31,3.1,1.8E-11,0.0,0.4)
$Br + HCHO \rightarrow HBr + CO + HO_2$	7.7E-12*EXP(-580./temp)
$CH_3Br + OH \rightarrow H_2O + Br$	2.35E-12*EXP(-1300./temp)
$BrO + ClO \rightarrow Br + OClO$	1.6E-12*EXP(430./temp)
$BrO + ClO \rightarrow Br + Cl + O_2$	2.9E-12*EXP(220./temp)
$BrO + ClO \rightarrow BrCl + O_2$	5.8E-13*EXP(170./temp)
$SO_2 + OH \rightarrow H_2SO_4 + HO_2$	k_3rd(temp,cair,3.3E-31,4.3,1.6E-12,0.,0.6)

Table S2. Heterogeneous reactions. Reaction rate constants are calculated by the PSC scheme of ICON-ART. The uptake coefficients of the different PSC types are taken from Sander et al. (2011), where not stated differently.

Reaction	γ_{STS}	γ_{NAT}	γ_{ice}
$N_2O_5 + H_2O \rightarrow 2\ HNO_3$	*(a)*	0.0004	0.027
$HOCl + HCl \rightarrow Cl_2 + H_2O$	*(a)*	0.1	0.2
$ClNO_3 + HCl \rightarrow Cl_2 + HNO_3$	*(a)*	0.2	0.3
$ClNO_3 + H_2O \rightarrow HOCl + HNO_3$	*(a)*	0.004	0.3
$N_2O_5 + HCl \rightarrow ClNO_2 + HNO_3$	*(a)*	0.003	0.03
$HOBr + HBr \rightarrow Br_2 + H_2O$	*(a)*	$0.1^{(b)}$	0.1
$BrNO_3 + H_2O \rightarrow HOBr + HNO_3$	*(a)*	$0.001^{(b)}$	0.26
$ClNO_3 + HBr \rightarrow BrCl + HNO_3$	*(a)*	0.3	0.3
$BrNO_3 + HCl \rightarrow BrCl + HNO_3$	*(a)*	$0.3^{(b)}$	0.26
$HOCl + HBr \rightarrow BrCl + H_2O$	*(a)*	$0.3^{(b)}$	$0.3^{(c)}$
$HOBr + HCl \rightarrow BrCl + H_2O$	*(a)*	$0.1^{(b)}$	0.3

$^{(a)}$ Parametrised according to Carslaw et al. (1995).

$^{(b)}$ In analogy to similar reactions, coming from Carslaw et al. (1995)

$^{(c)}$ In analogy to $HOBr + HCl$

Table S3. Photolytic reactions. Photolysis rates are calculated by the CloudJ module, incorporated in ICON-ART.

Reaction
$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$
$O_3 + h\nu \rightarrow O(^1D) + O_2$
$O_3 + h\nu \rightarrow O(^3P) + O_2$
$H_2O + h\nu \rightarrow H + OH$
$H_2O_2 + h\nu \rightarrow 2\ OH$
$N_2O + h\nu \rightarrow O(^1D) + N_2$
$NO_2 + h\nu \rightarrow NO + O(^3P)$
$NO + h\nu \rightarrow N + O(^3P)$
$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$
$NO_3 + h\nu \rightarrow NO + O_2$
$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$
$HNO_3 + h\nu \rightarrow NO_2 + OH$
$HNO_4 + h\nu \rightarrow .667\ NO_2 + .667\ HO_2 + .333\ NO_3 + .333\ OH$
$CH_3OOH + h\nu \rightarrow HCHO + OH + HO_2$
$HCHO + h\nu \rightarrow H_2 + CO$
$HCHO + h\nu \rightarrow H + CO + HO_2$
$CO_2 + h\nu \rightarrow CO + O(^3P)$
$CH_4 + h\nu \rightarrow CO + 0.31\ H + 0.69\ H_2 + 1.155\ H_2O$
$Cl_2 + h\nu \rightarrow Cl + Cl$
$Cl_2O_2 + h\nu \rightarrow 2\ Cl$
$OClO + h\nu \rightarrow ClO + O(^3P)$
$HOCl + h\nu \rightarrow OH + Cl$
$ClNO_2 + h\nu \rightarrow Cl + NO_2$
$ClNO_3 + h\nu \rightarrow Cl + NO_3$
$ClNO_3 + h\nu \rightarrow ClO + NO_2$
$CH_3Cl + h\nu \rightarrow Cl + CH_3O_2$
$CCl_4 + h\nu \rightarrow 4\ Cl$
$CH_3CCl_3 + h\nu \rightarrow 3\ Cl$
$CFCl_3 + h\nu \rightarrow 3\ Cl$
$CF_2Cl_2 + h\nu \rightarrow 2\ Cl$
$Br_2 + h\nu \rightarrow Br + Br$
$BrO + h\nu \rightarrow Br + O(^3P)$
$HOBr + h\nu \rightarrow Br + OH$
$BrNO_3 + h\nu \rightarrow 0.85\ Br + 0.85\ NO_3 + 0.15\ BrO + 0.15\ NO_2$
$CH_3Br + h\nu \rightarrow Br + CH_3O_2$
$CF_3Br + h\nu \rightarrow Br$
$BrCl + h\nu \rightarrow Br + Cl$
$CF_2ClBr + h\nu \rightarrow Br + Cl$

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