

Supplementary Material for

Short-Lived Halogen Sources and Chemistry in the Community Earth System Model v2 (CESM2-SLH)

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Supplementary Charts S1 and S2

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./\$PATH/components/cam/src/

chemistry

bulk aero

aerosol_depvel.F90

modal aero

aero_model.F90

mozart

chemistry.F90

clybryiy_fam.F90

gas_wetdep_opts.F90

iodine_emissions.F90

mo_chemini.F90

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pp trop strat mam4 slh

pp waccm tsmlt mam4 slh

physics

cam

physpkg.F90

Chart S1: Individual Fortran routines that have been updated within the CESM2-SLH CAM6-Cham folders. The individual files highlighted in bold are new files included in the model.

```

72 &cam_initfiles_nl
73   ncdata = '$PATH/FC.f19_f19_mg17.L32.cesm2.2-
74 asdbranch_slh_released.FCHIST_slh.Historical_SLH.cam.i.1980-01-01-00000.nc'
75 /
76 &chem_inparm
77   srf_emis_specifier = 'BENZENE -> $PATH/emissions-cmip6-ScenarioMIP_IAMC-AIM-ssp370-1-
78 1_BENZENE_anthro_surface_mol_175001-210101_0.9x1.25_c20190222.nc',
79 ...
80   'CHBR3 -> $PATH/emissions_CHBr3_chlorophyll_surface_Ordonez2012_flx1p15_cyclical_1850-
81 2100_1.9x2.5_c240804.nc',
82   'CH2BR2 -> $PATH/emissions_CH2Br2_chlorophyll_surface_Ordonez2012_flx1p15_cyclical_1850-
83 2100_1.9x2.5_c240804.nc',
84   'CH2BRCL-> $PATH/emissions_CH2BrCl_chlorophyll_surface_Ordonez2012_flx1p15_cyclical_1850-
85 2100_1.9x2.5_c240804.nc',
86   'CHBR2CL-> $PATH/emissions_CHBr2Cl_chlorophyll_surface_Ordonez2012_flx1p15_cyclical_1850-
87 2100_1.9x2.5_c240804.nc',
88   'CHBRCL2-> $PATH/emissions_CHBrCl2_chlorophyll_surface_Ordonez2012_flx1p15_cyclical_1850-
89 2100_1.9x2.5_c240804.nc',
90   'CH3I -> $PATH/emissions_CH3I_chlorophyll_surface_Ordonez2012_cyclical_1850-
91 2100_1.9x2.5_c240804.nc',
92   'CH2I2 -> $PATH/emissions_CH2I2_chlorophyll_surface_Ordonez2012_cyclical_1850-
93 2100_1.9x2.5_c240804.nc',
94   'CH2IBR -> $PATH/emissions_CH2IBr_chlorophyll_surface_Ordonez2012_cyclical_1850-
95 2100_1.9x2.5_c240804.nc',
96   'CH2ICL -> $PATH/emissions_CH2ICl_chlorophyll_surface_Ordonez2012_cyclical_1850-
97 2100_1.9x2.5_c240804.nc',
98   'CH2CL2 -> $PATH/emissions_CH2Cl2_NoNeg_surface_Claxton2020_flx1p15_serial_1850-
99 2100_1.9x2.5_c240722.nc',
100  'C2CL4 -> $PATH/emissions_C2Cl4_NoNeg_surface_Claxton2020_flx1p15_serial_1850-
101 2100_1.9x2.5_c240722.nc',
102  'I2 -> $PATH/emissions_I2_ocean_surface_PradosRoman2015_online_1850-2100_1.9x2.5_c240804.nc',
103  'HOI -> $PATH/emissions_HOI_ocean_surface_PradosRoman2015_online_1850-2100_1.9x2.5_c240804.nc'
104 /
105 &chem_surfvals_nl
106   flbc_file = '$PATH/LBC_1750-
107 2100_CMIP6_0p5degLat_HIST_c170126_SSP370_c180905_VSL_C1_CHCL3x1p15_C2H4CL2x1p15_c20240731.nc'
108   flbc_list = 'CCL4', 'CF2CLBR', 'CF3BR', 'CFC11', 'CFC113', 'CFC12', 'CH3BR', 'CH3CCL3', 'CH3CL', 'CH4',
109   'CO2', 'H2', 'HCFC22', 'N2O', 'CFC114', 'CFC115', 'HCFC141B', 'HCFC142B', 'H2402', 'OCS', 'SF6',
110   'CHCL3', 'C2H4CL2'
111 /
112 &prescribed_strataero_nl
113   prescribed_strataero_file = 'CESM_1949_2100_sad_V2_c130627.nc'
114 /
115 &wetdep_inparm
116   gas_wetdep_ice_uptake_list = 'HNO3', 'CLONO2', 'HCL', 'HOCL', 'BRNO2', 'CLNO2', 'I2O2', 'I2O3', 'I2O4'
117   gas_wetdep_list = 'ALKNIT', 'ALKOOH', ... , 'XYLOL', 'XYLOLOOH', 'CLNO2', 'BRNO2', 'BR2', 'BRCL',
118   'IONO2', 'INO2', 'HI', 'IO', 'OIO', 'ICL',
119   'IBR', 'I2O2', 'I2O3', 'I2O4', 'CHCL2O2', 'COCL2'
120 /
121 &drydep_inparm
122   drydep_list = 'ALKNIT', 'ALKOOH', ... , 'XYLOL', 'XYLOLOOH',
123   'CLONO2', 'HCL', 'HOCL', 'CLNO2', 'BRNO2', 'HBR', 'HOBR', 'BRNO2', 'BR2',
124   'IONO2', 'HI', 'HOI', 'INO2', 'I2O2', 'I2O3', 'I2O4', 'CHCL2O2', 'COCL2'
125 /
126 &slh_nl
127   SSadehal_ScalingFactor = 1.40; SSAhno3_ScalingFactor = 1.00; SSAn2o5_ScalingFactor = 1.00
128   LIQfraprx_ScalingFactor_I = 1.50; ICEfraprx_ScalingFactor_I = 1.30; ICEfraprx_ScalingFactor_Br = 1.00
129 /

```

Chart S2: User defined variables and parameters that must be updated in user_nl_cam to properly configure CESM2-SLH compsets. Example changes for the recommended *FCnudedg_slh* compset wit ($2^\circ \times 2^\circ$) resolution.

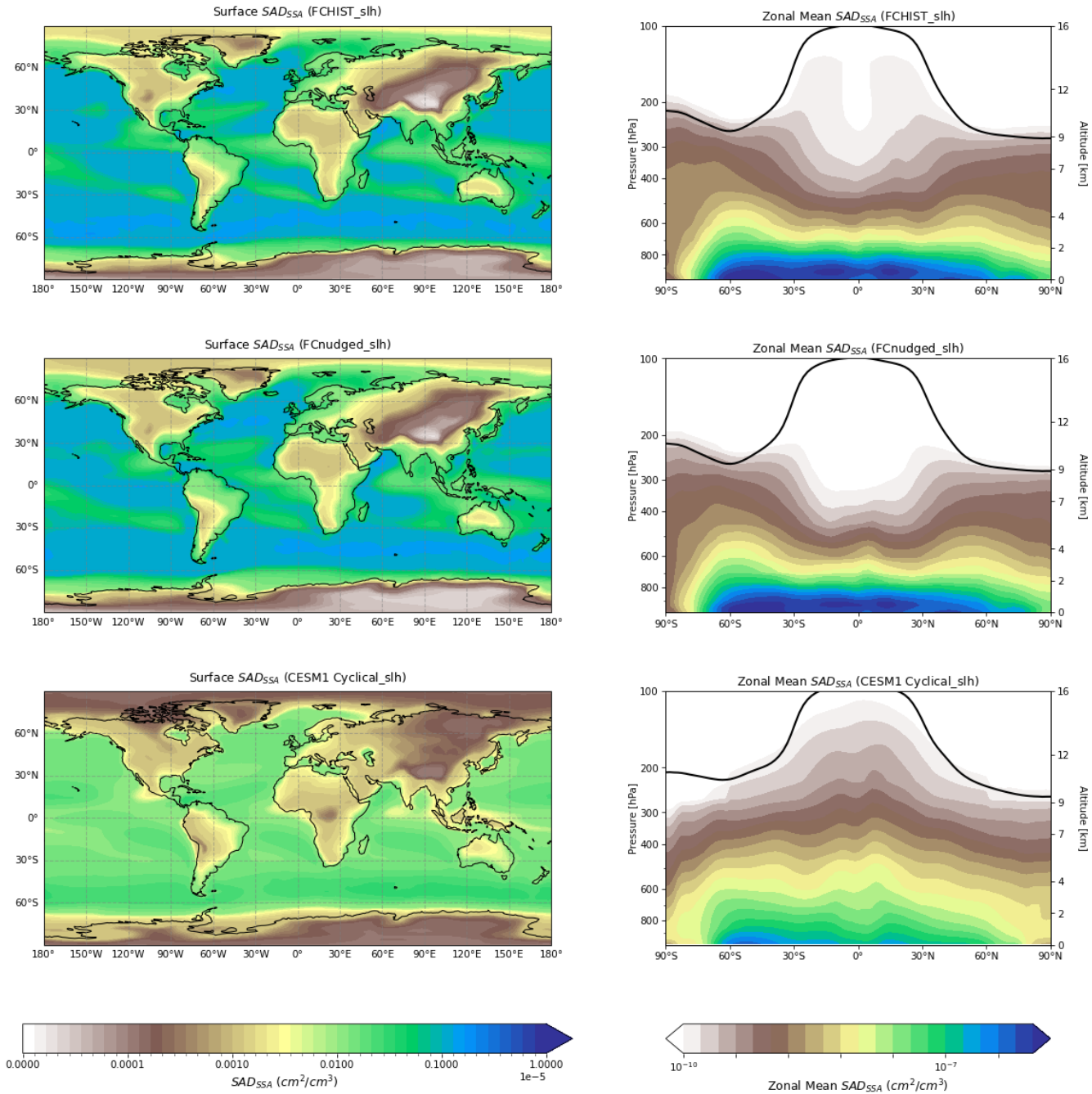
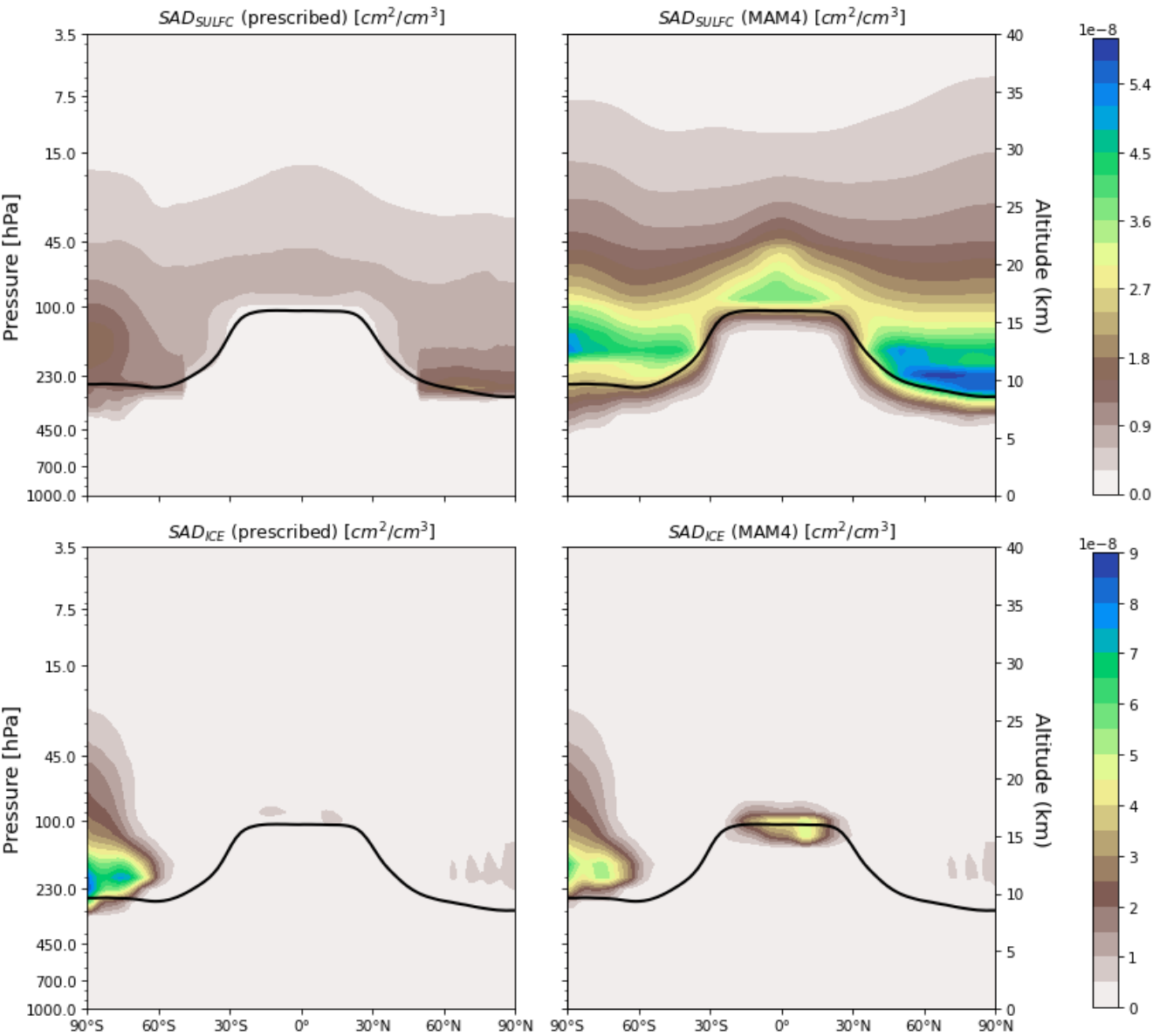


Figure S1: Annual mean distribution of surface area density for sea-salt aerosol (SAD_{SSA}) during present-day (2015-2020) for the *FCHIST_slh* (top row), *FCnudged_slh* (middle row) and *CESM1 Cyclical_slh* (bottom row) configurations. Left panels show the geographical variability within the model surface, while right columns show the tropospheric zonal average.



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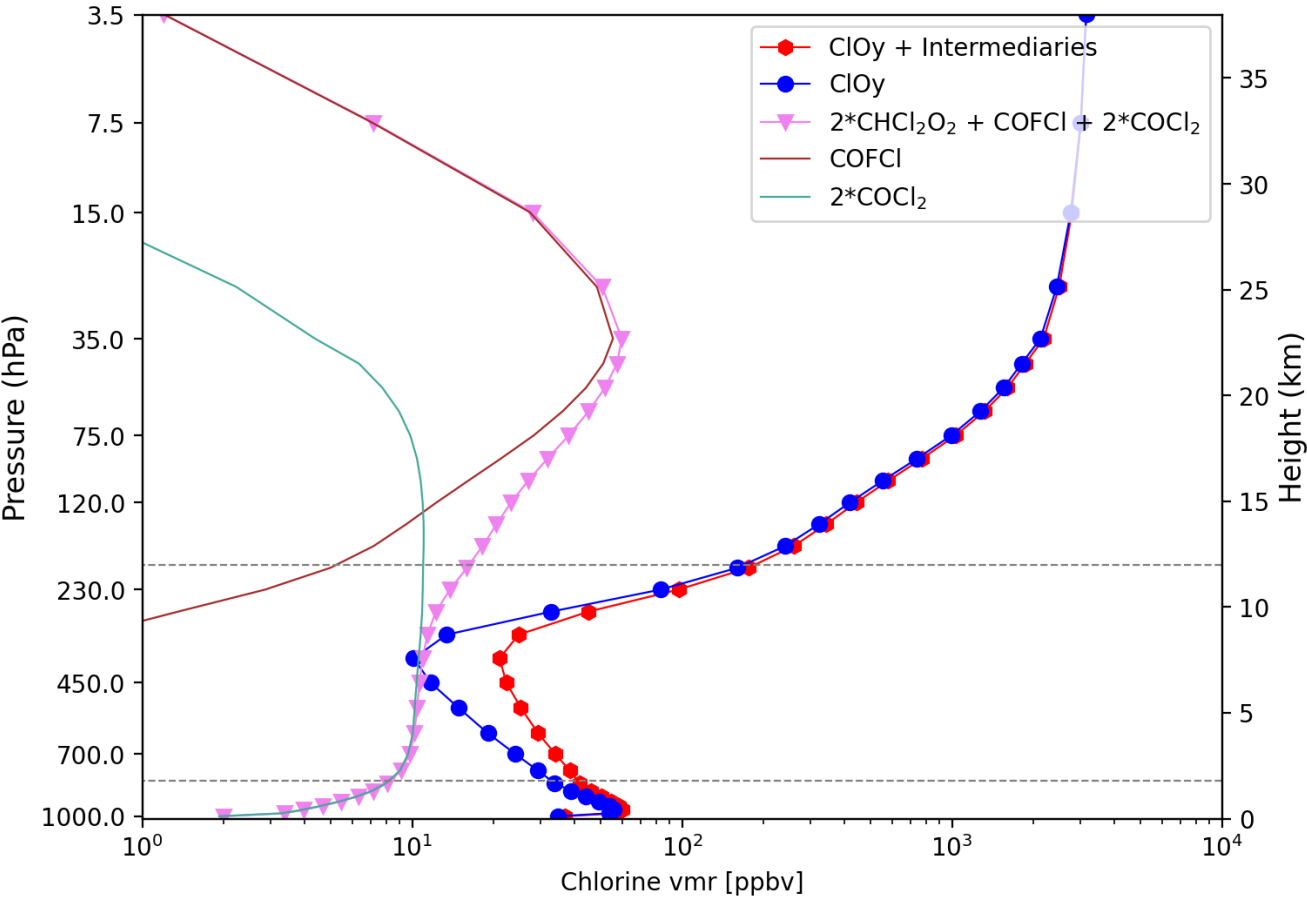
145

146

147

148

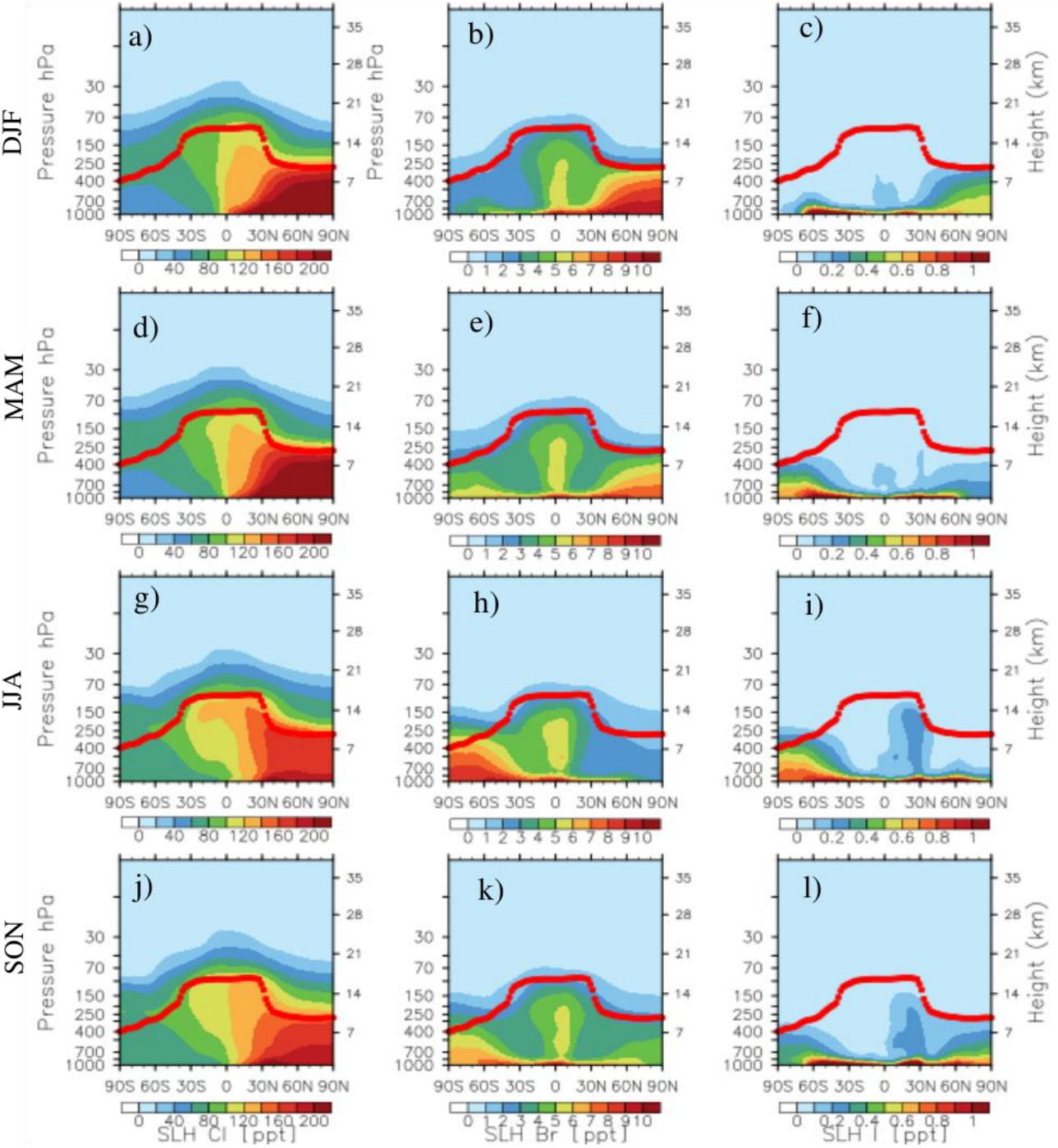
Figure S2: Present-day (2015-2020) zonal average of the Surface Area Density (SAD) for stratospheric sulphate (SAD_{SULFC} , top row) and stratospheric ice (SAD_{ICE} , bottom row) for different model configurations: (left) prescribed configuration and (right) online computation within the MAM4 aerosol scheme.



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151 **Figure S3: Global vertical profile of the contribution of intermediate chlorine species COCl₂, COFCl and CHCl₂O₂ to the total Cl_y**
152 **budget within the FCnuded_slh compset during present-day (2015-2020).**

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156 **Figure S4: Seasonality zonal average distribution of the very short-lived (VSL) organic (carbon bonded) halogen fraction during**
157 **present-day (2015-2020) for the *FCnudged_slh* compset. Left column shows chlorine (VSL_{Cl}), the center column shows bromine**
158 **(VSL_{Br}) and the right column shows iodine (VSL_I). The rows correspond to the different seasons, first row to december, january**
159 **and february ‘DJF’, second row to march, april and may ‘MAM’, third row to june, july and august ‘JJA’, and the fourth row to**
160 **september, october and november ‘SON’. The red-dotted line shows the mean model tropopause. See annual mean in Figure 4 (d,**
161 **e, f).**

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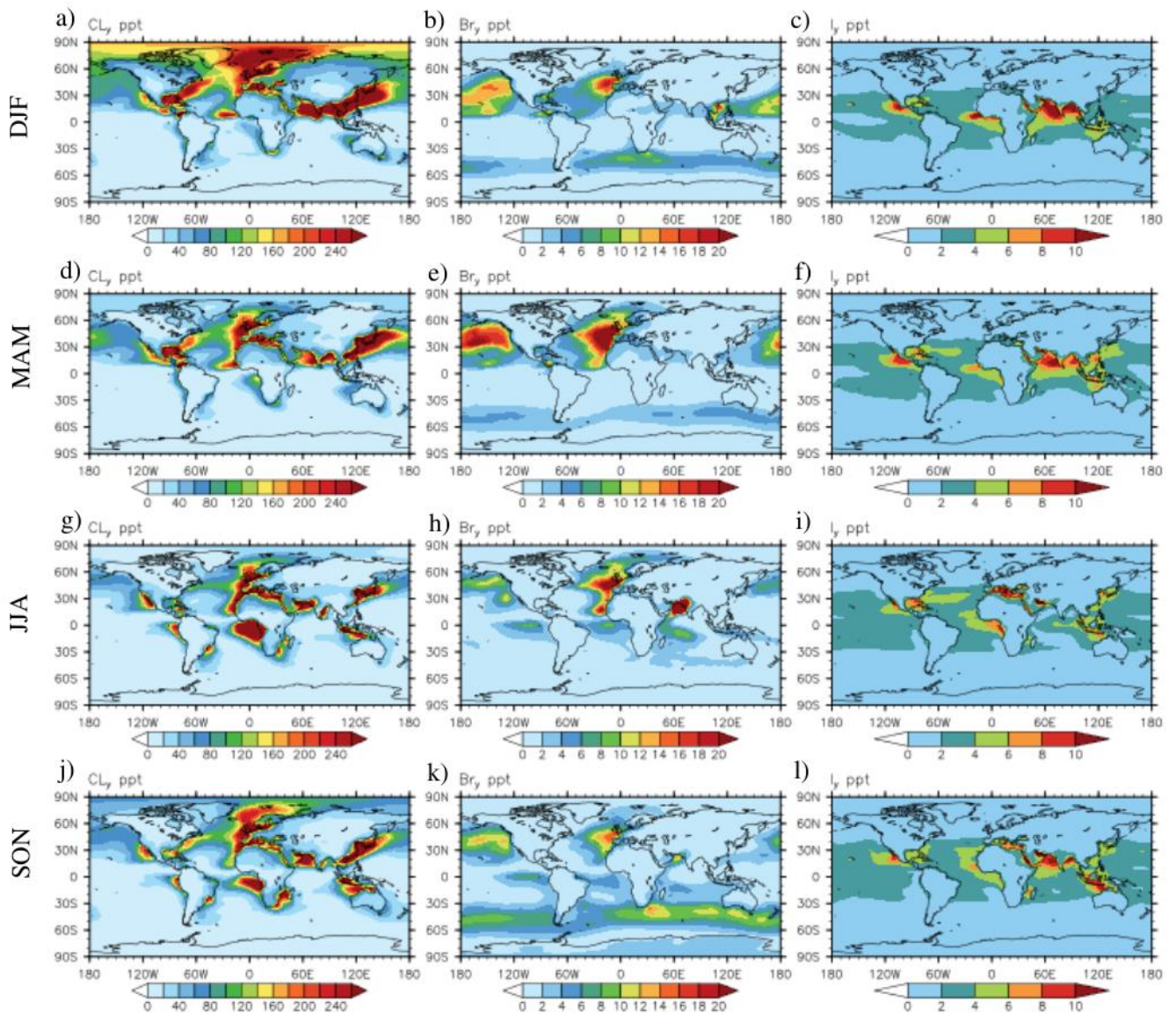
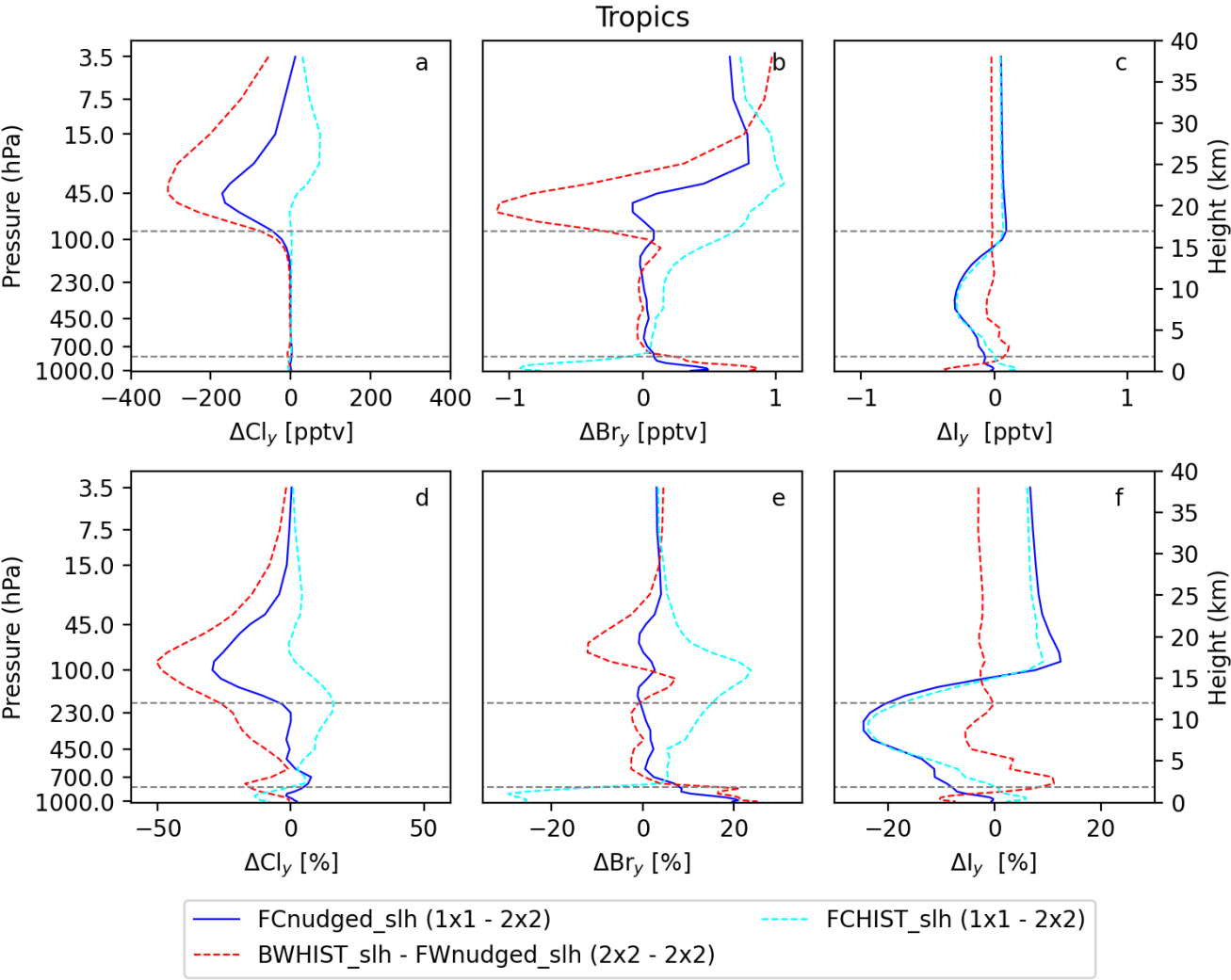


Figure S5: Geographical seasonal cycle of total inorganic halogen content during present-day (PD = 2015-2020) for the *FCnuded_slh* compset. Left column shows chlorine (CL), center column shows bromine (Br) and right column shows iodine (I). The rows correspond to the different seasons, first row to 'DJF', second row to 'MAM', third row to 'JJA' and fourth row to 'SON'. All magnitudes have been averaged within the boundary layer (from the model surface up to ~850 hPa). See annual mean in Figure 10 (d, e, f).



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173 **Figure S6. Percentage and Absolute differences of Vertical Profiles for the different compsets evaluated for the period 2000-2005 in**
174 **Tropics. Top row shows the absolute differences in pptv while bottom-row shows the corresponding percentage between the**
175 **compsets FCnudged_slh and FCnudged_1x1_slh in blue, between FCHIST_slh and FCHIST_1x1_slh compsets in light blue, and**
176 **between BWHIST_slh and FWnudged_slh compsets in dashed red for (a, d) chlorine (Cl_y), (b, e) bromine (Br_y) and (c, f) iodine.**

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Photolysis Reactions
$\text{CH}_2\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$
$\text{CHBr}_2\text{Cl} + h\nu \rightarrow 2^*\text{Br} + \text{Cl}$
$\text{CHBrCl}_2 + h\nu \rightarrow \text{Br} + 2^*\text{Cl}$
$\text{CH}_2\text{ICl} + h\nu \rightarrow \text{I} + \text{Cl}$
$\text{ICl} + h\nu \rightarrow \text{I} + \text{Cl}$
$\text{Cl}_2 + h\nu \rightarrow 2^*\text{Cl}$
$\text{ClO} + h\nu \rightarrow \text{Cl} + \text{O}$
$\text{OCIO} + h\nu \rightarrow \text{O} + \text{ClO}$
$\text{Cl}_2\text{O}_2 + h\nu \rightarrow 2^*\text{Cl}$
$\text{HOCl} + h\nu \rightarrow \text{OH} + \text{Cl}$
$\text{HCl} + h\nu \rightarrow \text{H} + \text{Cl}$
$\text{ClONO}_2 + h\nu \rightarrow \text{Cl} + \text{NO}_3$
$\text{ClONO}_2 + h\nu \rightarrow \text{ClO} + \text{NO}_2$
$\text{ClNO}_2 + h\nu \rightarrow \text{Cl} + \text{NO}_2$
$\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$
$\text{C}_2\text{Cl}_4 + h\nu \rightarrow 4^*\text{Cl}$
$\text{C}_2\text{H}_4\text{Cl}_2 + h\nu \rightarrow 2^*\text{Cl}$
$\text{CH}_2\text{Cl}_2 + h\nu \rightarrow 2^*\text{Cl}$
$\text{CH}_3\text{Cl} + h\nu \rightarrow \text{Cl} + \text{CH}_3\text{O}_2$
$\text{CHCl}_3 + h\nu \rightarrow \text{CHCl}_2\text{O}_2 + \text{Cl}$
$\text{ClNO}_2 + h\nu \rightarrow \text{Cl} + \text{NO}_2$
$\text{COCl}_2 + h\nu \rightarrow 2^*\text{Cl} + \text{CO}$
$\text{COFCl} + h\nu \rightarrow \text{F} + \text{Cl}$
$\text{CCl}_4 + h\nu \rightarrow 4^*\text{Cl}$
$\text{CH}_3\text{CCl}_3 + h\nu \rightarrow 3^*\text{Cl}$
$\text{CFC11} + h\nu \rightarrow 3^*\text{Cl}$
$\text{CFC12} + h\nu \rightarrow 2^*\text{Cl}$
$\text{CFC113} + h\nu \rightarrow 3^*\text{Cl}$
$\text{HCFC23} + h\nu \rightarrow \text{Cl}$
$\text{CH}_3\text{Br} + h\nu \rightarrow \text{Br} + \text{CH}_3\text{O}_2$
$\text{CF}_3\text{Br} + h\nu \rightarrow \text{Br}$
$\text{CF}_2\text{ClBr} + h\nu \rightarrow \text{Br} + \text{Cl}$
$\text{CFC114} + h\nu \rightarrow 2^*\text{Cl}$
$\text{CFC115} + h\nu \rightarrow \text{Cl}$
$\text{HCFC141B} + h\nu \rightarrow 2^*\text{Cl}$
$\text{HCFC142B} + h\nu \rightarrow \text{Cl}$
$\text{IBr} + h\nu \rightarrow \text{I} + \text{Br}$
$\text{CH}_2\text{IBr} + h\nu \rightarrow \text{I} + \text{Br}$
$\text{CHBr}_3 + h\nu \rightarrow 3^*\text{Br}$
$\text{CH}_2\text{Br}_2 + h\nu \rightarrow 2^*\text{Br}$
$\text{BrO} + h\nu \rightarrow \text{Br} + \text{O}$
$\text{HOBr} + h\nu \rightarrow \text{Br} + \text{OH}$
$\text{HBr} + h\nu \rightarrow \text{Br} + \text{H}$
$\text{BrONO}_2 + h\nu \rightarrow \text{Br} + \text{NO}_3$
$\text{BrONO}_2 + h\nu \rightarrow \text{BrO} + \text{NO}_2$
$\text{BrNO}_2 + h\nu \rightarrow \text{Br} + \text{NO}_2$
$\text{BrNO}_2 + h\nu \rightarrow \text{BrO} + \text{NO}$
$\text{Br}_2 + h\nu \rightarrow 2^*\text{Br}$
$\text{H}_{2402} + h\nu \rightarrow 2^*\text{Br}$
$\text{CH}_3\text{I} + h\nu \rightarrow \text{I} + \text{CH}_3\text{O}_2$
$\text{CH}_2\text{I}_2 + h\nu \rightarrow 2^*\text{I}$
$\text{I}_2 + h\nu \rightarrow 2^*\text{I}$
$\text{IO} + h\nu \rightarrow \text{I} + \text{O}$
$\text{OIO} + h\nu \rightarrow \text{I} + \text{O}_2$

$\text{INO} + h\nu \rightarrow \text{I} + \text{NO}$
$\text{INO}_2 + h\nu \rightarrow \text{I} + \text{NO}_2$
$\text{INO}_2 + h\nu \rightarrow \text{IO} + \text{NO}$
$\text{IONO}_2 + h\nu \rightarrow \text{I} + \text{NO}_3$
$\text{HOI} + h\nu \rightarrow \text{I} + \text{OH}$
$\text{HI} + h\nu \rightarrow \text{I} + \text{H}$
$\text{I}_2\text{O}_2 + h\nu \rightarrow \text{OIO} + \text{I}$
$\text{I}_2\text{O}_3 + h\nu \rightarrow \text{OIO} + \text{IO}$
$\text{I}_2\text{O}_4 + h\nu \rightarrow \text{OIO} + \text{OIO}$

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Odd-Oxygen Reactions	Rate
$O^1D + HCl \rightarrow Cl + OH$	9.90×10^{-11}
$O^1D + HCl \rightarrow ClO + H$	3.30×10^{-12}
$O^1D + HBr \rightarrow Br + OH$	9×10^{-11}
$O^1D + HBr \rightarrow BrO + H$	3×10^{-11}
$O^1D + HCN \rightarrow OH$	$7.70 \times 10^{-11} e^{(100/T)}$
$O^1D + CFC11 \rightarrow 2^*Cl + COFCl$	2.07×10^{-10}
$O^1D + CFC12 \rightarrow 2^*Cl + COF_2$	1.17×10^{-10}
$O^1D + CFC113 \rightarrow 2^*Cl + COFCl + COF_2$	2.088×10^{-10}
$O^1D + CFC114 \rightarrow 2^*Cl + 2^*COF_2$	1.17×10^{-10}
$O^1D + CFC115 \rightarrow Cl + F + 2^*COF_2$	4.644×10^{-11}
$O^1D + HCFC22 \rightarrow Cl + COF_2$	7.65×10^{-11}
$O^1D + HCFC141B \rightarrow Cl + COFCl$	1.794×10^{-10}
$O^1D + HCFC142B \rightarrow Cl + COF_2$	1.3×10^{-10}
$O^1D + CCl_4 \rightarrow 4^*Cl$	2.84×10^{-10}
$O^1D + COFCl \rightarrow F + Cl$	1.90×10^{-10}
$O^1D + CH_3Br \rightarrow Br$	1.8×10^{-10}
$O^1D + CF_2ClBr \rightarrow Cl + Br$	9.60×10^{-11}
$O^1D + CF_3Br \rightarrow Br + F + COF_2$	4.50×10^{-11}
$O^1D + H2402 \rightarrow 2^*Br + 2^*COF_2$	1.20×10^{-10}
$O^1D + CHBr_3 \rightarrow 3^*Br$	4.62×10^{-10}
$O^1D + CH_2Br_2 \rightarrow 2^*Br$	2.57×10^{-10}
Odd-Chlorine Reactions	Rate
$Cl + CH_2O \rightarrow HCl + HO_2 + CO$	$8.10 \times 10^{-11} e^{(-30/T)}$
$Cl + H_2 \rightarrow HCl + H$	$3.05 \times 10^{-11} e^{(-2270/T)}$
$Cl + H_2O_2 \rightarrow HCl + HO_2$	$1.10 \times 10^{-11} e^{(-980/T)}$
$Cl + HO_2 \rightarrow HCl + O_2$	$1.40 \times 10^{-11} e^{(270/T)}$
$Cl + HO_2 \rightarrow OH + ClO$	$3.60 \times 10^{-11} e^{(-375/T)}$
$ClNO_2 + OH \rightarrow HOCl + NO_2$	$2.40 \times 10^{-12} e^{(-1250/T)}$
$Cl + O_3 \rightarrow ClO + O_2$	$2.30 \times 10^{-11} e^{(-200/T)}$
$ClO + CH_3O_2 \rightarrow Cl + HO_2 + CH_2O$	$3.3 \times 10^{-12} e^{(-115/T)}$
$ClO + ClO \rightarrow 2^*Cl + O_2$	$3.00 \times 10^{-11} e^{(-2450/T)}$
$ClO + ClO \rightarrow Cl_2 + O_2$	$1.00 \times 10^{-12} e^{(-1590/T)}$
$ClO + ClO \rightarrow Cl + OCIO$	$3.50 \times 10^{-13} e^{(-1370/T)}$
$ClO + HO_2 \rightarrow O_2 + HOCl$	$2.60 \times 10^{-12} e^{(290/T)}$
$ClO + NO \rightarrow NO_2 + Cl$	$6.40 \times 10^{-12} e^{(290/T)}$
$ClONO_2 + Cl \rightarrow Cl_2 + NO_3$	$6.50 \times 10^{-12} e^{(135/T)}$
$ClONO_2 + O \rightarrow ClO + NO_3$	$3.60 \times 10^{-12} e^{(-840/T)}$
$ClONO_2 + OH \rightarrow HOCl + NO_3$	$1.20 \times 10^{-12} e^{(-330/T)}$
$ClO + O \rightarrow Cl + O_2$	$2.80 \times 10^{-11} e^{(85/T)}$
$ClO + OH \rightarrow Cl + HO_2$	$7.40 \times 10^{-12} e^{(270/T)}$
$ClO + OH \rightarrow HCl + O_2$	$6.00 \times 10^{-13} e^{(230/T)}$
$HCl + O \rightarrow Cl + OH$	$1.00 \times 10^{-11} e^{(-3300/T)}$
$HCl + OH \rightarrow H_2O + Cl$	$1.80 \times 10^{-12} e^{(-250/T)}$
$HOCl + Cl \rightarrow HCl + ClO$	$3.40 \times 10^{-12} e^{(-130/T)}$
$HOCl + O \rightarrow ClO + OH$	1.70×10^{-13}
$HOCl + OH \rightarrow H_2O + ClO$	$3.00 \times 10^{-12} e^{(-500/T)}$
Odd bromine reactions	Rate
$Br_2 + OH \rightarrow HOBr + Br$	$2.10 \times 10^{-11} e^{(240/T)}$
$Br + O_3 \rightarrow BrO + O_2$	$1.60 \times 10^{-11} e^{(-780/T)}$
$Br + HO_2 \rightarrow HBr + O_2$	$4.80 \times 10^{-12} e^{(-310/T)}$
$Br + CH_2O \rightarrow HBr + HO_2 + CO$	$1.70 \times 10^{-11} e^{(-800/T)}$
$BrO + BrO \rightarrow 2^*Br + O_2$	$1.50 \times 10^{-12} e^{(230/T)}$
$BrO + ClO \rightarrow Br + OCIO$	$9.50 \times 10^{-13} e^{(550/T)}$
$BrO + ClO \rightarrow Br + Cl + O_2$	$2.30 \times 10^{-12} e^{(260/T)}$
$BrO + ClO \rightarrow BrCl + O_2$	$4.10 \times 10^{-13} e^{(290/T)}$
$BrO + NO \rightarrow Br + NO_2$	$8.80 \times 10^{-12} e^{(260/T)}$

$\text{BrONO}_2 + \text{Br} \rightarrow \text{Br}_2 + \text{NO}_3$	$1.78 \times 10^{-11} \text{e}^{(365/\text{T})}$
$\text{BrONO}_2 + \text{Cl} \rightarrow \text{BrCl} + \text{NO}_3$	$6.28 \times 10^{-11} \text{e}^{(215/\text{T})}$
$\text{BrONO}_2 + \text{O} \rightarrow \text{BrO} + \text{NO}_3$	$1.90 \times 10^{-11} \text{e}^{(215/\text{T})}$
$\text{BrO} + \text{O} \rightarrow \text{Br} + \text{O}_2$	$1.90 \times 10^{-11} \text{e}^{(230/\text{T})}$
$\text{BrO} + \text{OH} \rightarrow \text{Br} + \text{HO}_2$	$1.70 \times 10^{-11} \text{e}^{(250/\text{T})}$
$\text{HBr} + \text{OH} \rightarrow \text{Br} + \text{H}_2\text{O}$	$5.50 \times 10^{-12} \text{e}^{(200/\text{T})}$
$\text{HBr} + \text{O} \rightarrow \text{Br} + \text{OH}$	$5.80 \times 10^{-12} \text{e}^{(-1500/\text{T})}$
$\text{HOBr} + \text{O} \rightarrow \text{BrO} + \text{OH}$	$1.20 \times 10^{-10} \text{e}^{(-430/\text{T})}$
Odd iodine reaction	Rate
$\text{HI} + \text{NO}_3 \rightarrow \text{I} + \text{HNO}_3$	$1.30 \times 10^{-12} \text{e}^{(-1830/\text{T})}$
$\text{HOI} + \text{OH} \rightarrow \text{IO} + \text{H}_2\text{O}$	2.00×10^{-13}
$\text{I}_2 + \text{NO}_3 \rightarrow \text{I} + \text{IONO}_2$	1.50×10^{-12}
$\text{I}_2 + \text{O} \rightarrow \text{IO} + \text{I}$	1.25×10^{-10}
$\text{I}_2 + \text{OH} \rightarrow \text{HOI} + \text{I}$	1.80×10^{-10}
$\text{I} + \text{BrO} \rightarrow \text{IO} + \text{Br}$	1.44×10^{-11}
$\text{I} + \text{HO}_2 \rightarrow \text{HI} + \text{O}_2$	$1.50 \times 10^{-11} \text{e}^{(-1090/\text{T})}$
$\text{I} + \text{IONO}_2 \rightarrow \text{I}_2 + \text{NO}_3$	$9.10 \times 10^{-11} \text{e}^{(-146/\text{T})}$
$\text{INO}_2 + \text{INO}_2 \rightarrow \text{I}_2 + 2^*\text{NO}_2$	$4.70 \times 10^{-13} \text{e}^{(-1670/\text{T})}$
$\text{INO}_2 \rightarrow \text{I} + \text{NO}_2$	$1.008 \times 10^{18} \text{e}^{(-13670/\text{T})}$
$\text{I} + \text{NO}_3 \rightarrow \text{IO} + \text{NO}_2$	1.00×10^{-10}
$\text{INO} + \text{INO} \rightarrow \text{I}_2 + 2^*\text{NO}$	$8.40 \times 10^{-11} \text{e}^{(-2620/\text{T})}$
$\text{I} + \text{O}_3 \rightarrow \text{IO} + \text{O}_2$	$2.10 \times 10^{-11} \text{e}^{(-830/\text{T})}$
$\text{IO} + \text{Br} \rightarrow \text{I} + \text{BrO}$	2.49×10^{-11}
$\text{IO} + \text{BrO} \rightarrow \text{Br} + \text{I} + \text{O}_2$	$0.30 \times 10^{-11} \text{e}^{(510/\text{T})}$
$\text{IO} + \text{BrO} \rightarrow \text{Br} + \text{OIO}$	$1.20 \times 10^{-11} \text{e}^{(510/\text{T})}$
$\text{IO} + \text{ClO} \rightarrow \text{I} + \text{OCIO}$	$2.585 \times 10^{-12} \text{e}^{(280/\text{T})}$
$\text{IO} + \text{ClO} \rightarrow \text{I} + \text{Cl} + \text{O}_2$	$1.175 \times 10^{-12} \text{e}^{(280/\text{T})}$
$\text{IO} + \text{ClO} \rightarrow \text{ICl} + \text{O}_2$	$0.940 \times 10^{-12} \text{e}^{(280/\text{T})}$
$\text{IO} + \text{NO} \rightarrow \text{I} + \text{NO}_2$	$7.15 \times 10^{-12} \text{e}^{(300/\text{T})}$
$\text{IO} + \text{HO}_2 \rightarrow \text{HOI} + \text{O}_2$	$1.30 \times 10^{-11} \text{e}^{(570/\text{T})}$
$\text{IO} + \text{NO}_3 \rightarrow \text{OIO} + \text{NO}_2$	9.00×10^{-12}
$\text{IO} + \text{O} \rightarrow \text{I} + \text{O}_2$	1.40×10^{-10}
$\text{IO} + \text{O}_3 \rightarrow \text{OIO} + \text{O}_2$	3.60×10^{-16}
$\text{IO} + \text{OH} \rightarrow \text{HO}_2 + \text{I}$	1.00×10^{-10}
$\text{OH} + \text{HI} \rightarrow \text{I} + \text{H}_2\text{O}$	$1.60 \times 10^{-11} \text{e}^{(440/\text{T})}$
$\text{OIO} + \text{NO} \rightarrow \text{IO} + \text{NO}_2$	$1.10 \times 10^{-12} \text{e}^{(542/\text{T})}$
$\text{HOI} + \text{NO}_3 \rightarrow \text{IO} + \text{HNO}_3$	
$\text{I}_2\text{O}_2 \rightarrow \text{OIO} + \text{I}$	
$\text{I}_2\text{O}_3 \rightarrow \text{IO} + \text{IO}$	
$\text{I}_2\text{O}_4 \rightarrow 2^*\text{OIO}$	
$\text{IO} + \text{IO} \rightarrow \text{OIO} + \text{I}$	
$\text{IO} + \text{IO} \rightarrow \text{I}_2\text{O}_2$	
$\text{IO} + \text{OIO} \rightarrow \text{I}_2\text{O}_3$	
$\text{OIO} + \text{OIO} \rightarrow \text{I}_2\text{O}_4$	
VSL halocarbon degradation	Rate
$\text{C}_2\text{Cl}_4 + \text{OH} \rightarrow 0.47^* \text{COCl}_2 + 3.06^* \text{Cl}$	$4.7 \times 10^{-12} \text{e}^{(-990/\text{T})}$
$\text{C}_2\text{H}_4\text{Cl}_2 + \text{Cl} \rightarrow 2^* \text{Cl} + \text{HCl}$	1.30×10^{-12}
$\text{C}_2\text{H}_4\text{Cl}_2 + \text{OH} \rightarrow 2^* \text{Cl} + \text{H}_2\text{O}$	$1.14 \times 10^{-11} \text{e}^{(-1150/\text{T})}$
$\text{CH}_2\text{Br}_2 + \text{Cl} \rightarrow 2^* \text{Br} + \text{HCl}$	$6.30 \times 10^{-12} \text{e}^{(-800/\text{T})}$
$\text{CH}_2\text{Br}_2 + \text{OH} \rightarrow 2^* \text{Br} + \text{H}_2\text{O}$	$2.00 \times 10^{-12} \text{e}^{(-840/\text{T})}$
$\text{CH}_2\text{BrCl} + \text{OH} \rightarrow \text{Br} + \text{Cl}$	$2.10 \times 10^{-12} \text{e}^{(-880/\text{T})}$
$\text{CH}_2\text{Cl}_2 + \text{Cl} \rightarrow \text{CHCl}_2\text{O}_2 + \text{HCl}$	$7.40 \times 10^{-12} \text{e}^{(-910/\text{T})}$
$\text{CH}_2\text{Cl}_2 + \text{OH} \rightarrow \text{CHCl}_2\text{O}_2 + \text{H}_2\text{O}$	$1.90 \times 10^{-12} \text{e}^{(-880/\text{T})}$
$\text{CH}_3\text{Br} + \text{Cl} \rightarrow \text{HCl} + \text{HO}_2 + \text{Br}$	$1.46 \times 10^{-11} \text{e}^{(-1040/\text{T})}$
$\text{CH}_3\text{Br} + \text{OH} \rightarrow \text{Br} + \text{H}_2\text{O} + \text{HO}_2$	$1.42 \times 10^{-12} \text{e}^{(-1150/\text{T})}$
$\text{CH}_3\text{CCl}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + 3^* \text{Cl}$	$1.64 \times 10^{-12} \text{e}^{(-1520/\text{T})}$
$\text{CH}_3\text{Cl} + \text{Cl} \rightarrow \text{HO}_2 + \text{CO} + 2^* \text{HCl}$	$2.03 \times 10^{-11} \text{e}^{(-1110/\text{T})}$
$\text{CH}_3\text{Cl} + \text{Cl} \rightarrow \text{HO}_2 + \text{CO} + 2^* \text{HCl}$	$2.03 \times 10^{-11} \text{e}^{(-1200/\text{T})}$
$\text{CH}_3\text{I} + \text{Cl} \rightarrow \text{I} + \text{HCl} + \text{HO}_2$	$2.90 \times 10^{-11} \text{e}^{(-1000/\text{T})}$
$\text{CH}_3\text{I} + \text{OH} \rightarrow \text{I} + \text{H}_2\text{O} + \text{HO}_2$	$2.90 \times 10^{-12} \text{e}^{(-1100/\text{T})}$

$\text{CHBr}_2\text{Cl} + \text{OH} \rightarrow 2^*\text{Br} + \text{Cl}$	$9.00 \times 10^{-13} \text{e}^{(-420/T)}$
$\text{CHBr}_3 + \text{Cl} \rightarrow 3^*\text{Br} + \text{HCl}$	$4.85 \times 10^{-12} \text{e}^{(-850/T)}$
$\text{CHBr}_3 + \text{OH} \rightarrow 3^*\text{Br}$	$9.00 \times 10^{-13} \text{e}^{(-360/T)}$
$\text{CHBrCl}_2 + \text{OH} \rightarrow \text{Br} + 2^*\text{Cl}$	$9.40 \times 10^{-13} \text{e}^{(-510/T)}$
$\text{CHCl}_2\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow 2^*\text{Cl} + 2^*\text{HO}_2 + \text{CH}_2\text{O} + \text{CO}$	1.20×10^{-12}
$\text{CHCl}_2\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{COCl}_2 + \text{CO} + \text{H}_2\text{O}$	8.00×10^{-13}
$\text{CHCl}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{COCl}_2 + \text{H}_2\text{O} + \text{O}_2$	$3.92 \times 10^{-13} \text{e}^{(700/T)}$
$\text{CHCl}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O} + \text{CO} + \text{Cl} + \text{HOCl}$	$1.68 \times 10^{-13} \text{e}^{(700/T)}$
$\text{CHCl}_2\text{O}_2 + \text{NO} \rightarrow \text{H}_2\text{O} + 2^*\text{Cl} + \text{NO}_2 + \text{CO}$	$4.05 \times 10^{-12} \text{e}^{(360/T)}$
$\text{CHCl}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{H}_2\text{O} + 2^*\text{Cl} + \text{NO}_2 + \text{CO}$	2.30×10^{-12}
$\text{CHCl}_3 + \text{Cl} \rightarrow \text{COCl}_2 + \text{Cl} + \text{HCl}$	$3.30 \times 10^{-12} \text{e}^{(-990/T)}$
$\text{CHCl}_2\text{O}_2 + \text{OH} \rightarrow \text{COCl}_2 + \text{Cl} + \text{H}_2\text{O}$	$2.20 \times 10^{-12} \text{e}^{(-920/T)}$
$\text{HCFC141B} + \text{OH} \rightarrow \text{Cl} + \text{COFCl}$	$1.25 \times 10^{-12} \text{e}^{(-1600/T)}$
$\text{HCFC142B} + \text{OH} \rightarrow \text{Cl} + 2^*\text{COF}_2$	$1.30 \times 10^{-12} \text{e}^{(-1770/T)}$
$\text{HCFC22} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Cl} + \text{COF}_2$	$1.05 \times 10^{-12} \text{e}^{(-1600/T)}$
Sulphur and Carbon	
$\text{DMS} + \text{BrO} \rightarrow \text{SO}_2 + \text{Br}$	$1.00 \times 10^{-14} \text{e}^{(950/T)}$
$\text{DMS} + \text{Cl} \rightarrow \text{sink}$	3.30×10^{-10}
$\text{DMS} + \text{Cl} \rightarrow \text{SO}_2 + \text{HCl}$	$9.40 \times 10^{-11} \text{e}^{(190/T)}$
$\text{DMS} + \text{IO} \rightarrow \text{SO}_2 + \text{I}$	$3.20 \times 10^{-13} \text{e}^{(-925/T)}$
C2	
$\text{C}_2\text{H}_6 + \text{Cl} \rightarrow \text{HCl} + \text{C}_2\text{H}_5\text{O}_2$	$7.20 \times 10^{-11} \text{e}^{(-70/T)}$
$\text{CH}_4 + \text{Cl} \rightarrow \text{CH}_3\text{O}_2 + \text{HCl}$	$7.10 \times 10^{-12} \text{e}^{(-1270/T)}$

Temperature (T) is expressed in K.

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187 **Table S3: Termolecular Reactions separated by halogen family**

Odd-Chlorine Reactions	Rate
$\text{Cl} + \text{NO}_2 + \text{M} \rightarrow \text{ClNO}_2 + \text{M}$	troe: $k_0 = 1.80 \times 10^{-31} \times (300/T)^{2.0}$ $k_i = 1.0 \times 10^{-10} \times (300/T)^{1.0}$, $f=0.6$ $2.40 \times 10^{-12} e^{(-1250/T)}$
$\text{ClO} + \text{NO}_2 + \text{M} \rightarrow \text{ClONO}_2 + \text{M}$	troe: $k_0 = 1.80 \times 10^{-31} \times (300/T)^{3.4}$ $k_i = 1.5 \times 10^{-11} \times (300/T)^{1.9}$, $f=0.6$
$\text{ClO} + \text{ClO} + \text{M} \rightarrow \text{Cl}_2\text{O}_2 + \text{M}$	troe: $k_0 = 1.90 \times 10^{-32} \times (300/T)^{3.6}$ $k_i = 3.7 \times 10^{-12} \times (300/T)^{1.6}$, $f=0.6$
Odd bromine reactions	Rate
$\text{Br} + \text{NO}_2 + \text{M} \rightarrow \text{BrNO}_2 + \text{M}$	troe: $k_0 = 4.20 \times 10^{-31} \times (300/T)^{2.4}$ $k_i = 2.7 \times 10^{-11}$, $f=0.6$
$\text{BrO} + \text{NO}_2 + \text{M} \rightarrow \text{BrONO}_2 + \text{M}$	troe: $k_0 = 5.20 \times 10^{-31} \times (300/T)^{3.2}$ $k_i = 6.9 \times 10^{-12} \times (300/T)^{2.9}$, $f=0.6$
Odd iodine reaction	Rate
$\text{I} + \text{NO}_2 + \text{M} \rightarrow \text{INO}_2 + \text{M}$	troe: $k_0 = 3.00 \times 10^{-31} \times (300/T)$ $k_i = 6.6 \times 10^{-11}$, $f=0.6$
$\text{I} + \text{NO} + \text{M} \rightarrow \text{INO} + \text{M}$	troe: $k_0 = 1.80 \times 10^{-32} \times (300/T)^{1.0}$ $k_i = 1.7 \times 10^{-11}$, $f=0.6$
$\text{IO} + \text{NO}_2 + \text{M} \rightarrow \text{IONO}_2 + \text{M}$	troe: $k_0 = 6.50 \times 10^{-31} \times (300/T)^{3.5}$ $K_i = 7.6 \times 10^{-12} \times (300/T)^{1.5}$, $f=0.6$
Organic halogen reaction with Cl, OH	Rate
$\text{C}_2\text{Cl}_4 + \text{Cl} + \text{M} \rightarrow 5^*\text{Cl}$	troe: $k_0 = 1.40 \times 10^{-28} \times (300/T)^{8.5}$ $K_i = 4.0 \times 10^{-11} \times (300/T)^{1.2}$, $f=0.6$
$\text{C}_2\text{H}_4 + \text{Cl} + \text{M} \rightarrow \text{Cl} + \text{M}$	troe: $k_0 = 1.60 \times 10^{-29} \times (300/T)^{3.3}$ $k_i = 3.1 \times 10^{-10} \times (300/T)^{1.0}$, $f=0.6$

188 Temperature (T) is expressed in K, air density (M) in molecules/cm³, k_i and k_0 in cm³/molec/s.

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