

Supplementary Material for

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

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Supplementary Figures S1 to S9

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Supplementary Charts S1 to S3

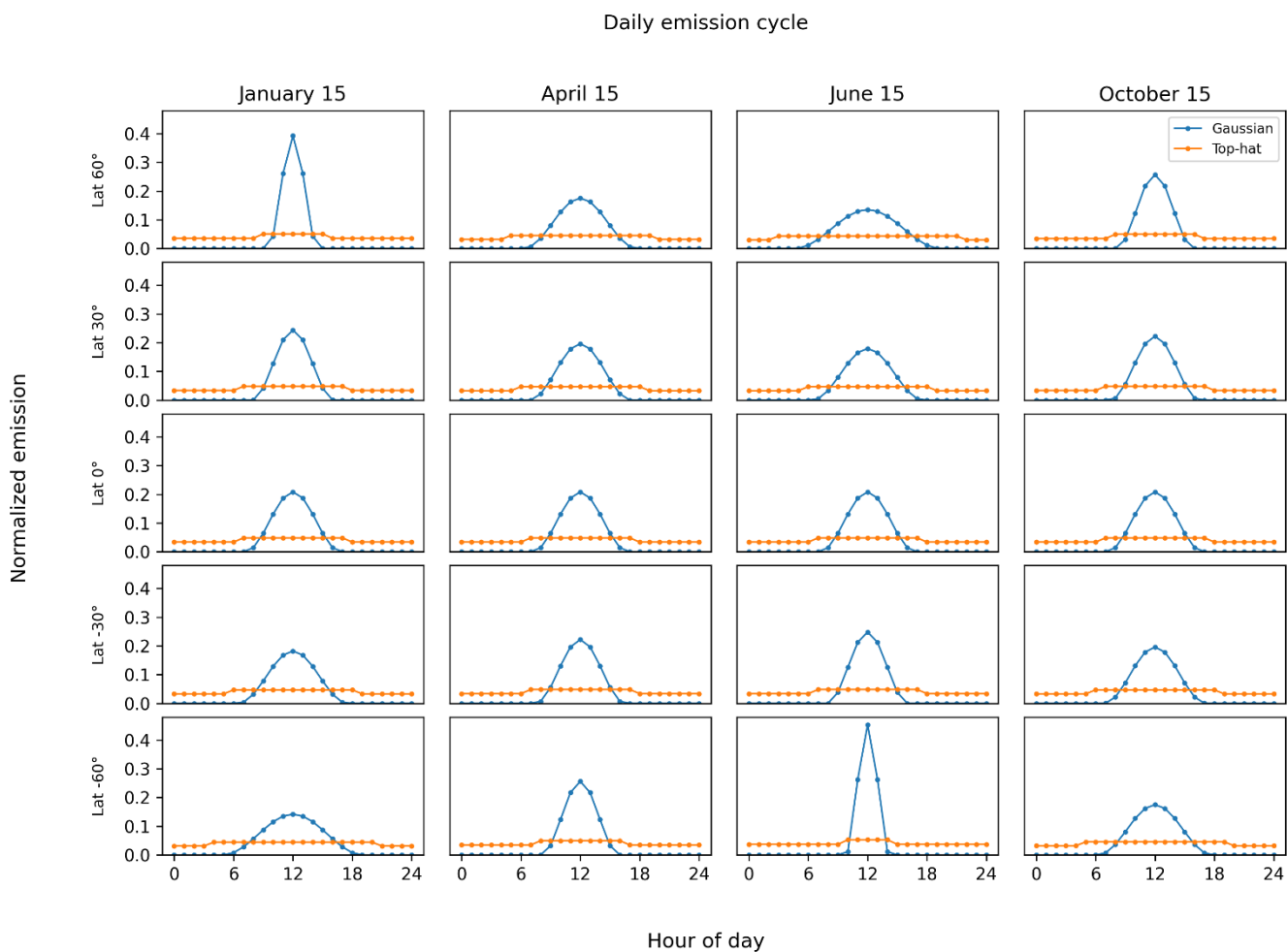


Figure S1: Hourly diurnal variation applied to all oceanic VSL halocarbon emissions considered in the in Ordóñez et al. (2012) inventory. Either the Gaussian or the top-hat temporal profiles are multiplied by the monthly offline emission strength interpolated to each day of the year, and considers the natural daily solar cycle at each specific latitude and longitude.

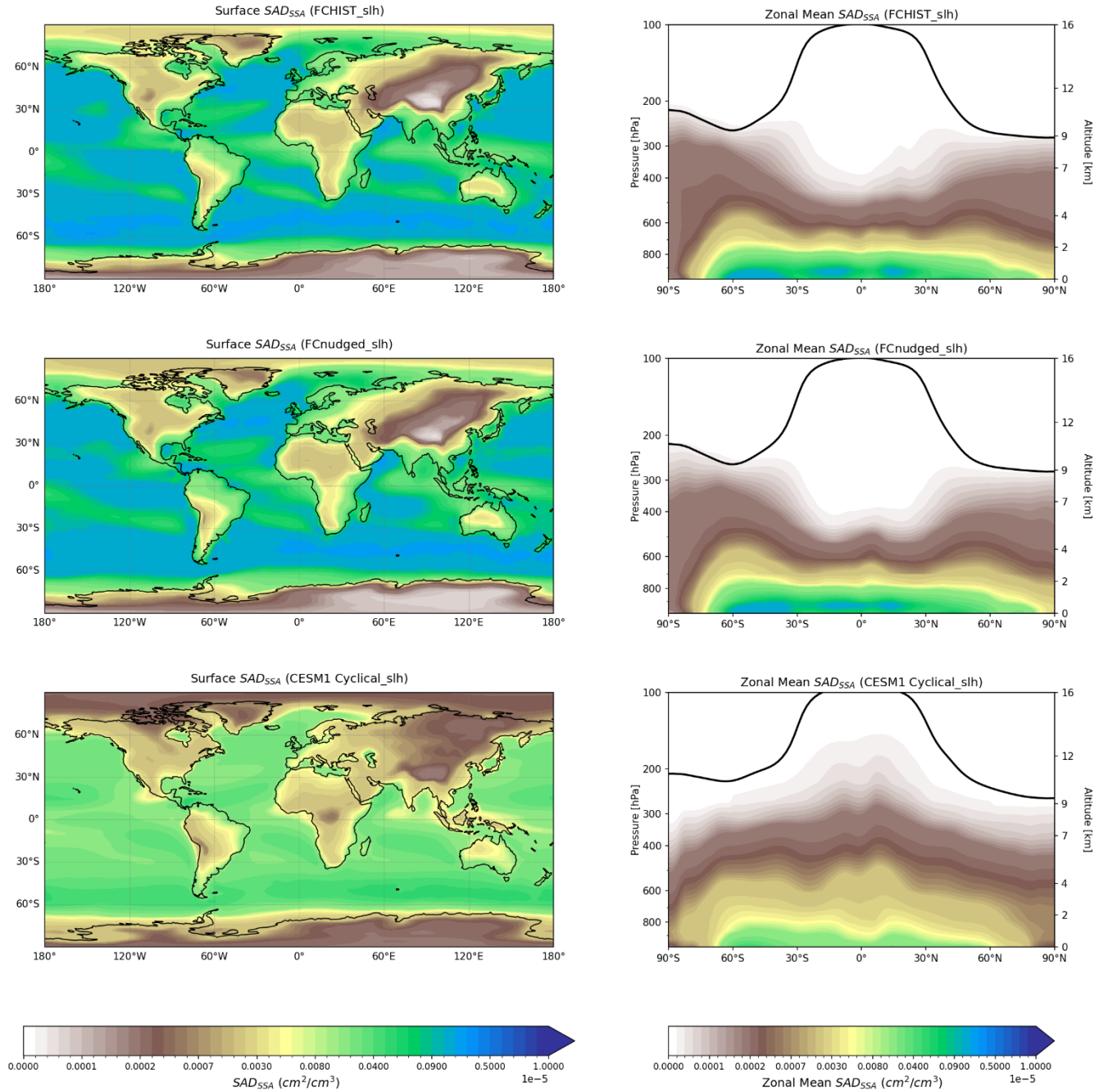


Figure S2: Annual mean distribution of surface area density for sea-salt aerosol (SAD_{SSA}) during present-day (2015-2020) for the CC-SLH [2×2-hst] (top row), CC-SLH [2×2-ndg] (middle row) and CESM1-SLH [SL23] (bottom row) experiments. Left panels show the geographical variability within the model surface, while right columns show the tropospheric zonal average. The black solid line in right panels shows the mean model tropopause.

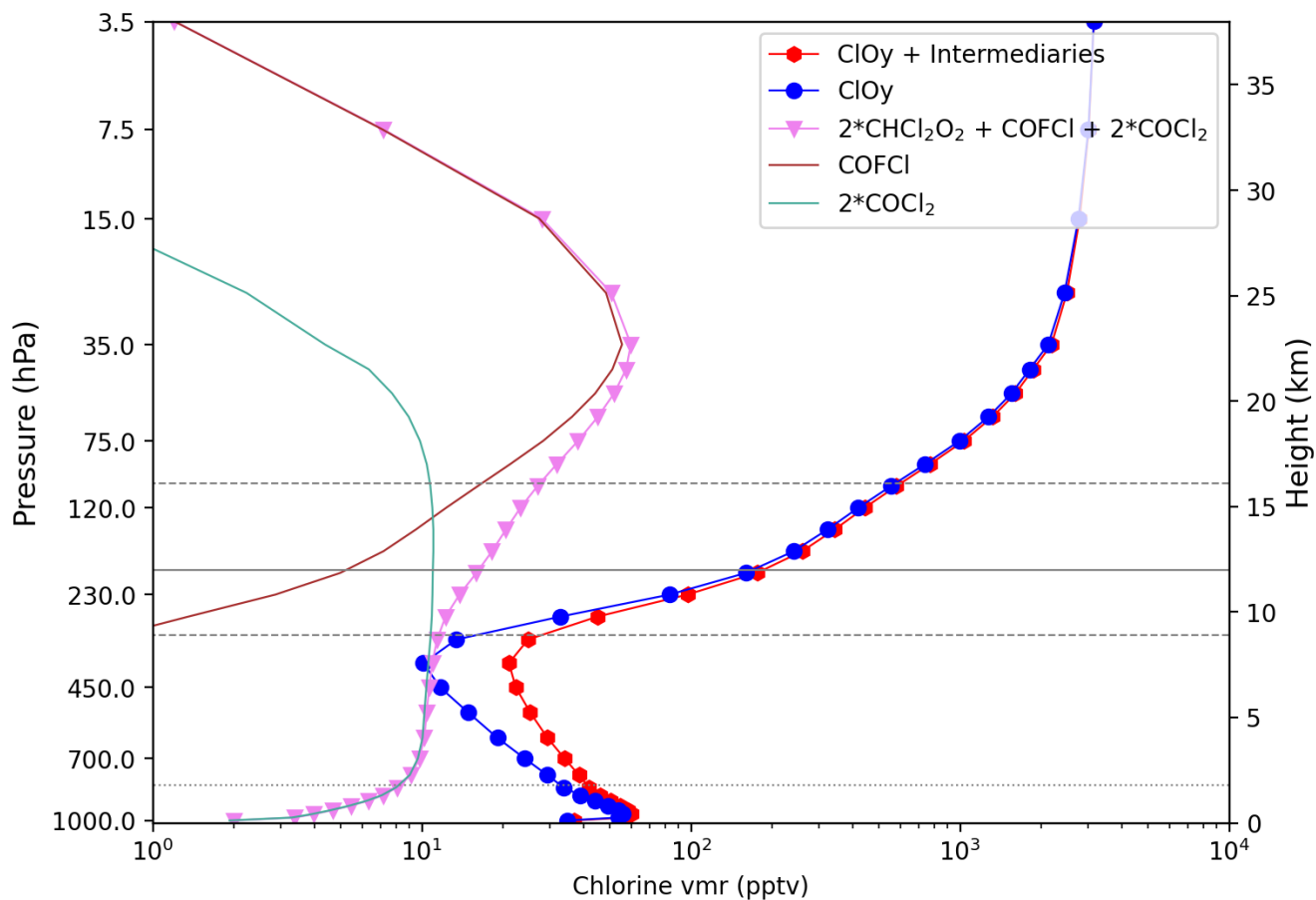


Figure S3: Global vertical profile of the contribution of intermediate chlorine species COCl_2 , COFCl and CHCl_2O_2 to the total Cl_y budget for the CC-SLH [2×2-ndg] experiment during present-day (2015-2020). The horizontal solid and dashed lines show the global mean tropopause height $\pm$ standard deviation, while the horizontal dotted line corresponds to $P = 850$ hPa

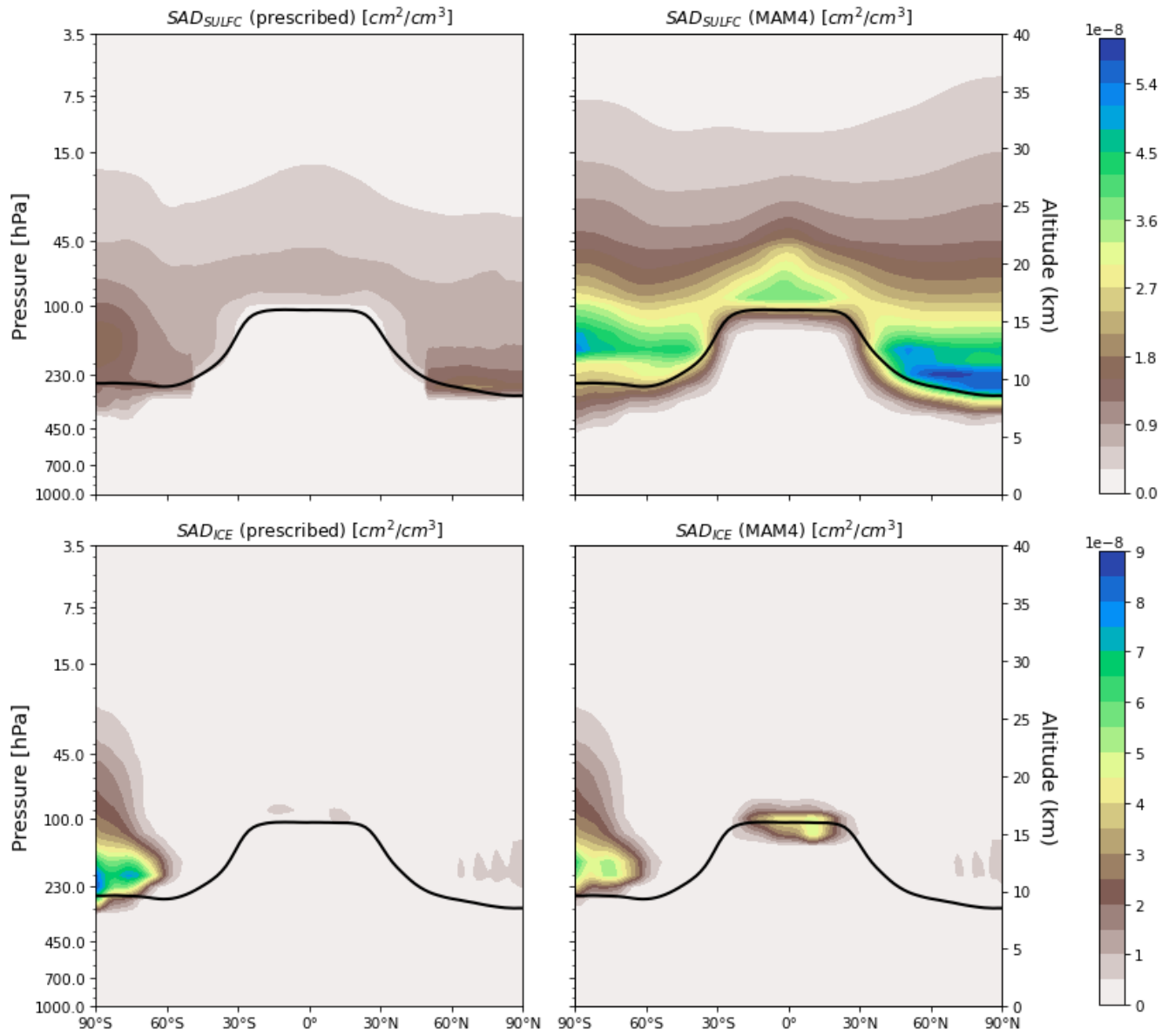


Figure S4: Present-day (2015-2020) zonal average of the Surface Area Density (SAD) for stratospheric sulphate (SAD_{SULFC} , top row) and stratospheric ice (SAD_{ICE} , bottom row) for different CC-SLH [2x2-ndg] sensitivities: (left) prescribed configuration and (right) online computation within the MAM4 aerosol scheme. The black solid line shows the mean model tropopause.

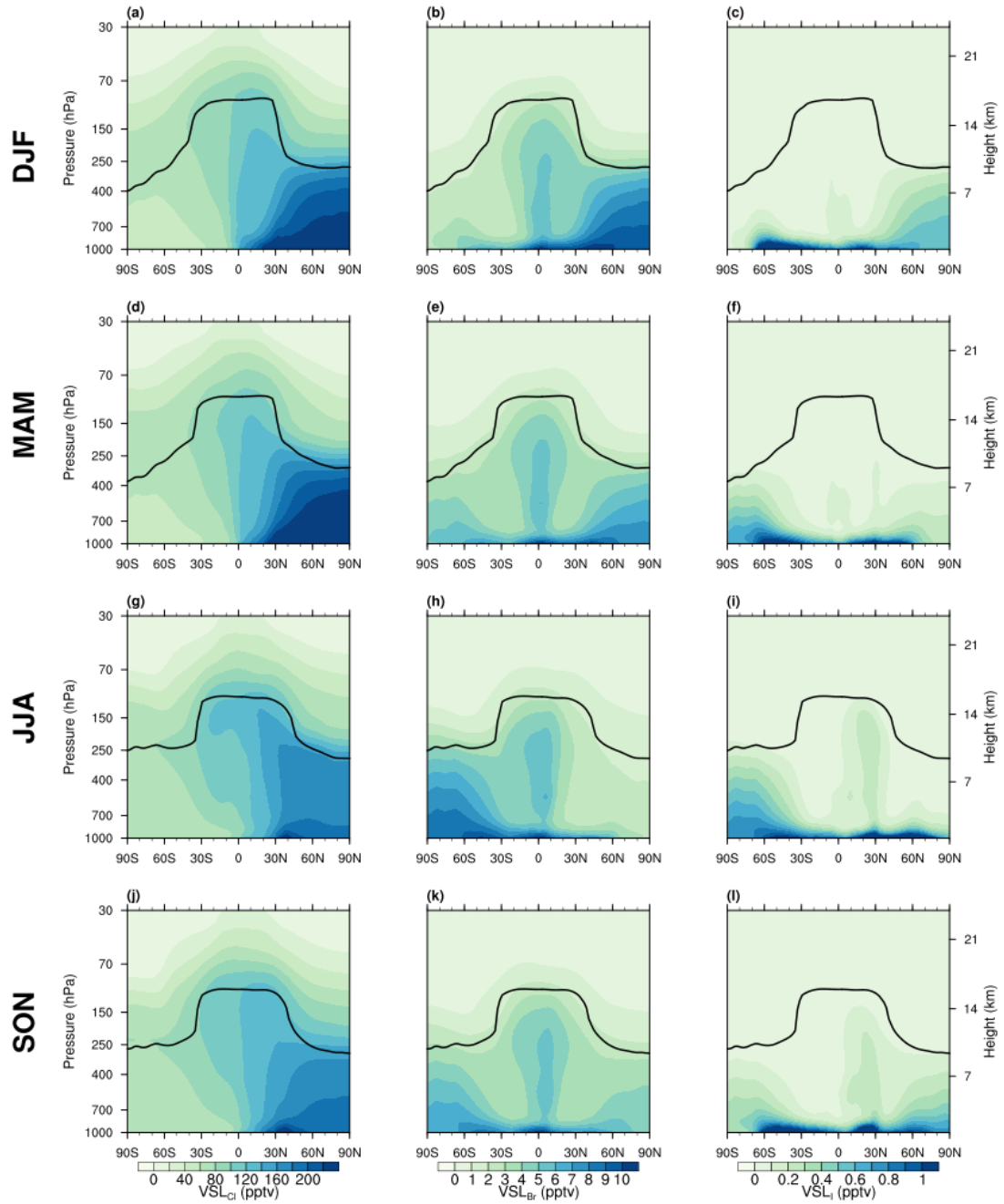


Figure S5: Seasonality zonal average distribution of the very short-lived (VSL) organic halogen fraction during present-day (2015-2020) for the CC-SLH [2×2-ndg] experiment. Left column shows chlorine (VSL_{Cl}), the center column shows bromine (VSL_{Br}) and the right column shows iodine (VSL_I). The rows correspond to the different seasons, first row for december, january and february ‘DJF’, second row for march, april and may ‘MAM’, third row for june, july and august ‘JJA’, and the fourth row for september, october and november ‘SON’. The black solid line shows the mean model tropopause. See annual mean in Figure 7c-e.

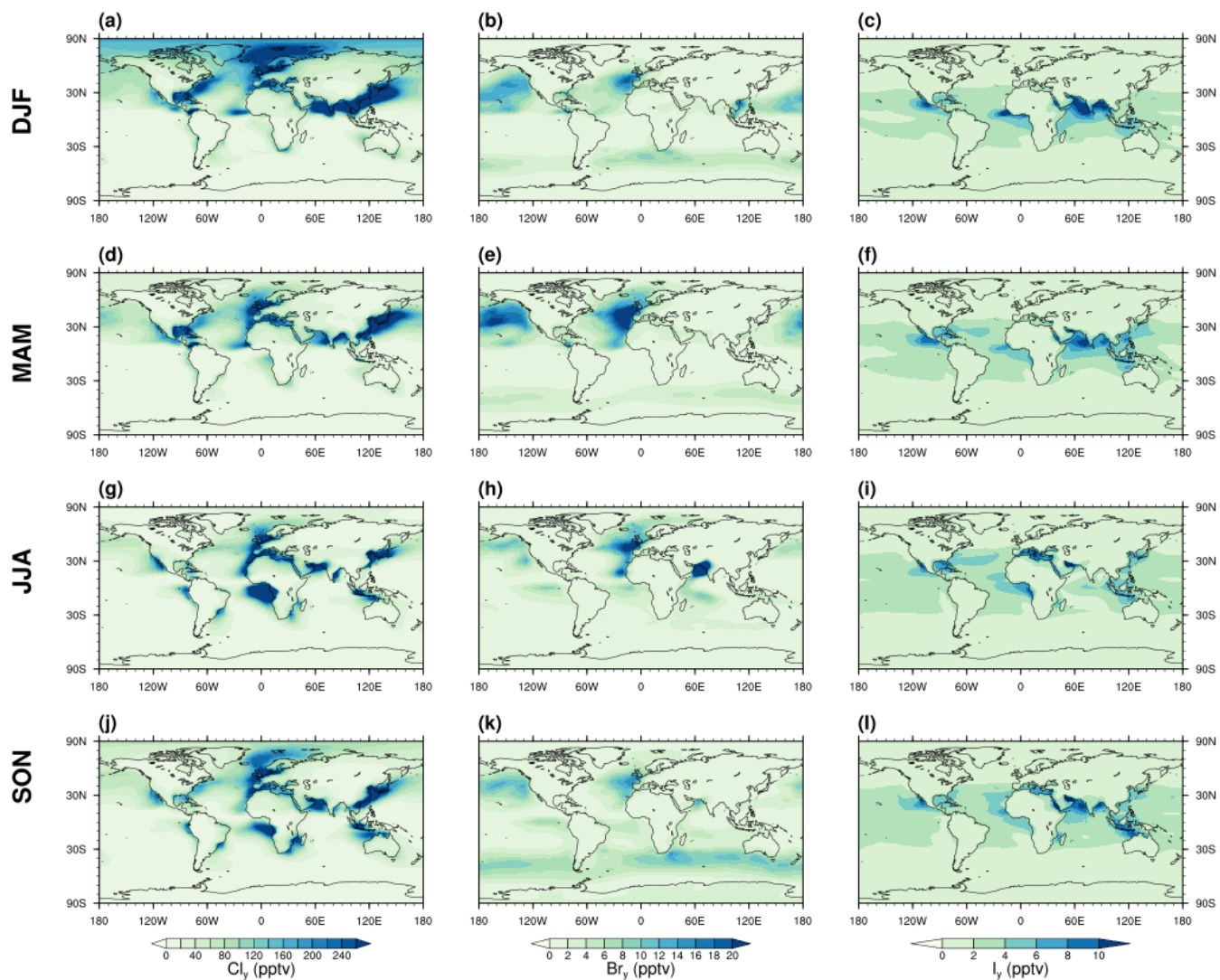


Figure S6: Geographical seasonal cycle of total inorganic halogen content during present-day (PD = 2015-2020) for the CC-SLH [2×2-ndg] experiment. Left column shows chlorine (Cl_y), center column shows bromine (Br_y) and right column shows iodine (I_y). The rows correspond to the different seasons, first row for ‘DJF’, second row for ‘MAM’, third row for ‘JJA’ and fourth row for ‘SON’. All magnitudes have been averaged from the model surface up to ~850 hPa. See annual mean in Figure 11d-f.

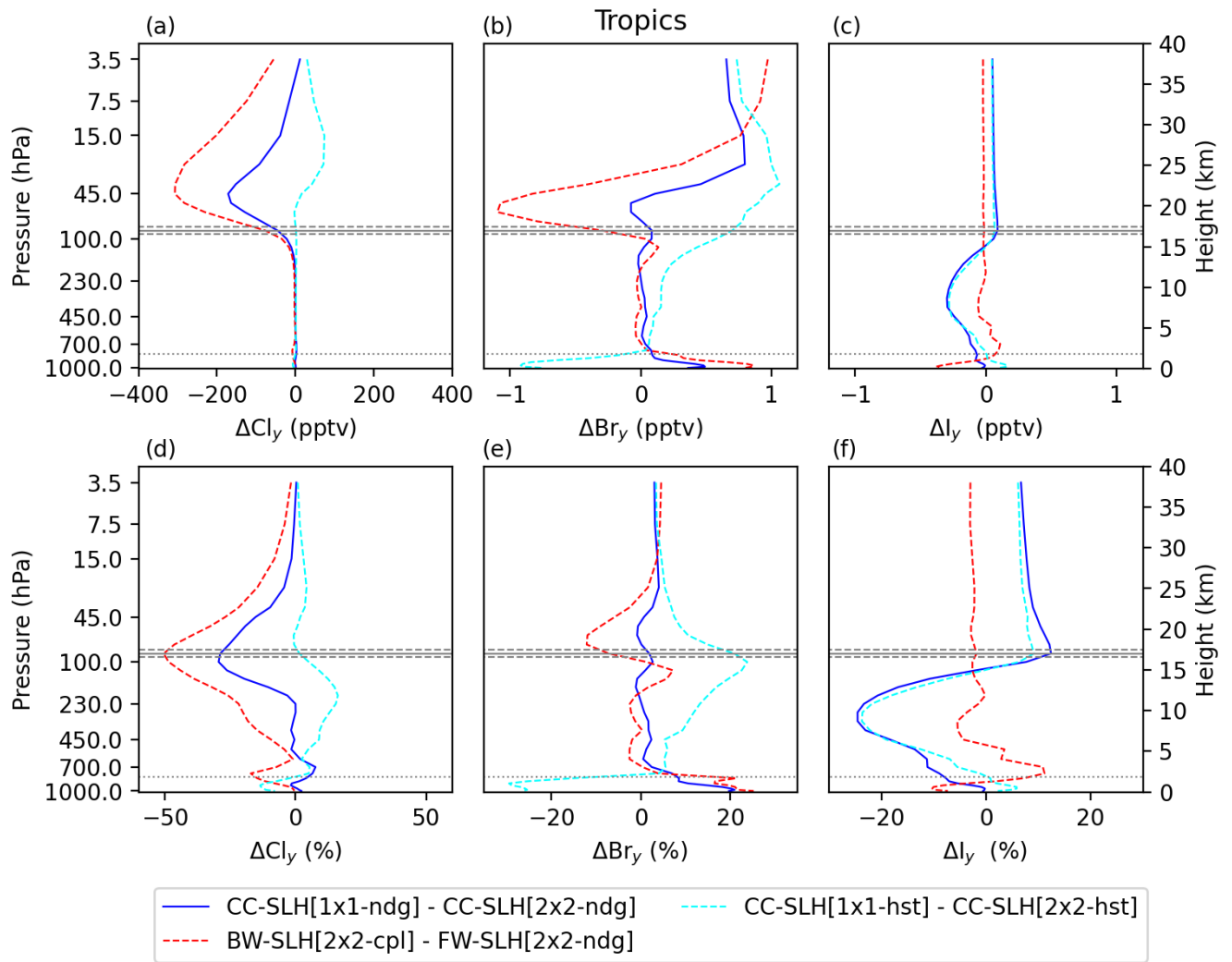


Figure S7. Percentage and Absolute differences of Tropical Vertical Profiles between the different experiments for the period 2000-2005. Top row shows the absolute differences in pptv while bottom-row shows the corresponding percentage between pair of experiments with different resolution and/or ocean coupling for (a, d) chlorine (Cl_y), (b, e) bromine (Br_y) and (c, f) iodine.

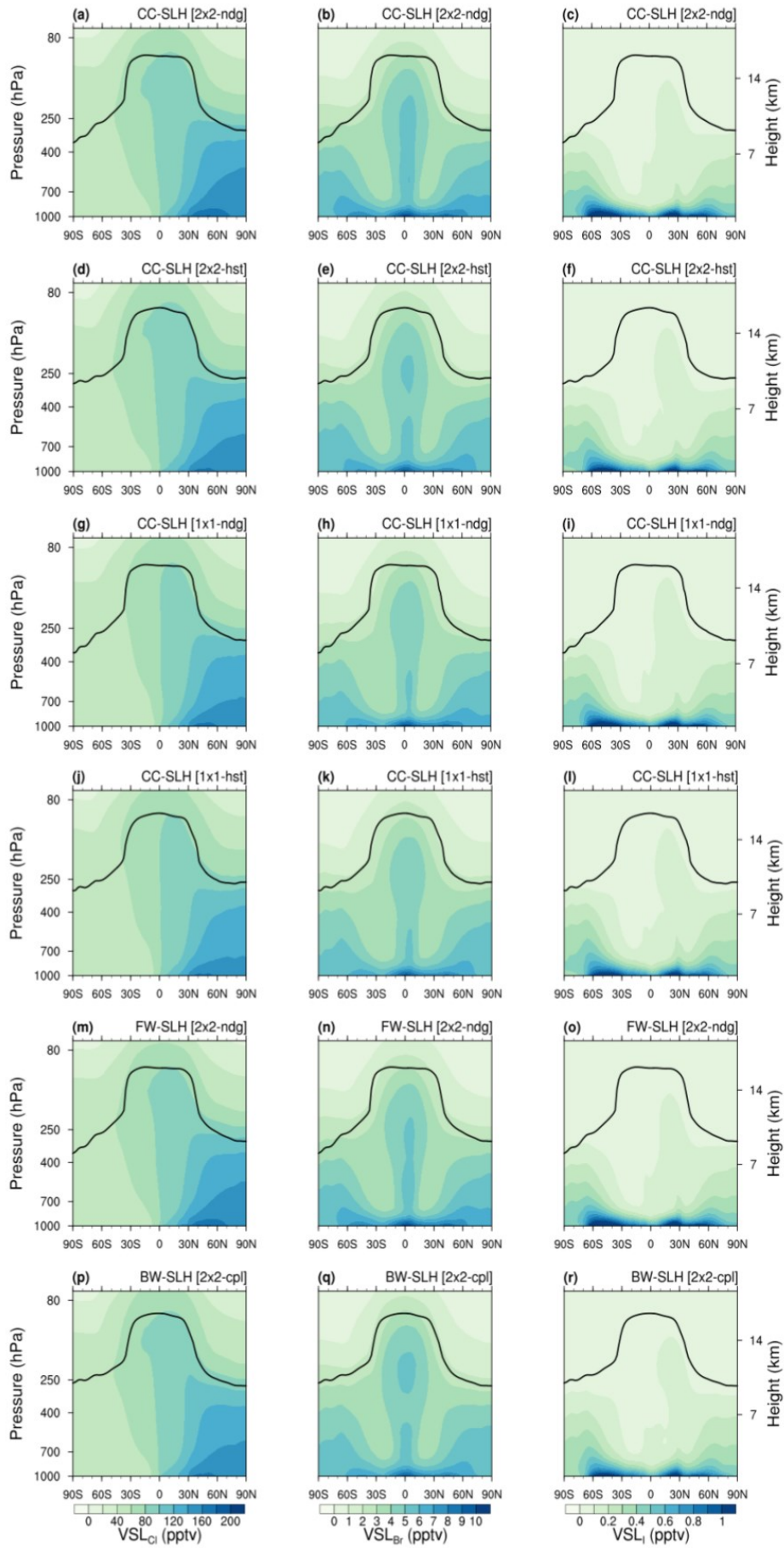


Figure S8: Comparison of VSL abundance between different CESM2-SLH compsets and resolutions. Left, middle and right columns show the zonal average distribution for chlorine (VSL_{Cl}), bromine (VSL_{Br}) and iodine (VSL_I), respectively. Each row presents results for individual CESM2-SLH experiments: CC-SLH [2x2-ndg] (1st row), CC-SLH [2x2-hst] (2nd row), CC-SLH [1x1-ndg] (3rd row), CC-SLH [1x1-hst] (4th row), FW-SLH [2x2-ndg] (5th row) and BW-SLH [2x2-cpl] (6th row). All output correspond to the annual mean for the 2000–2005 period. The black solid line shows the mean model tropopause.

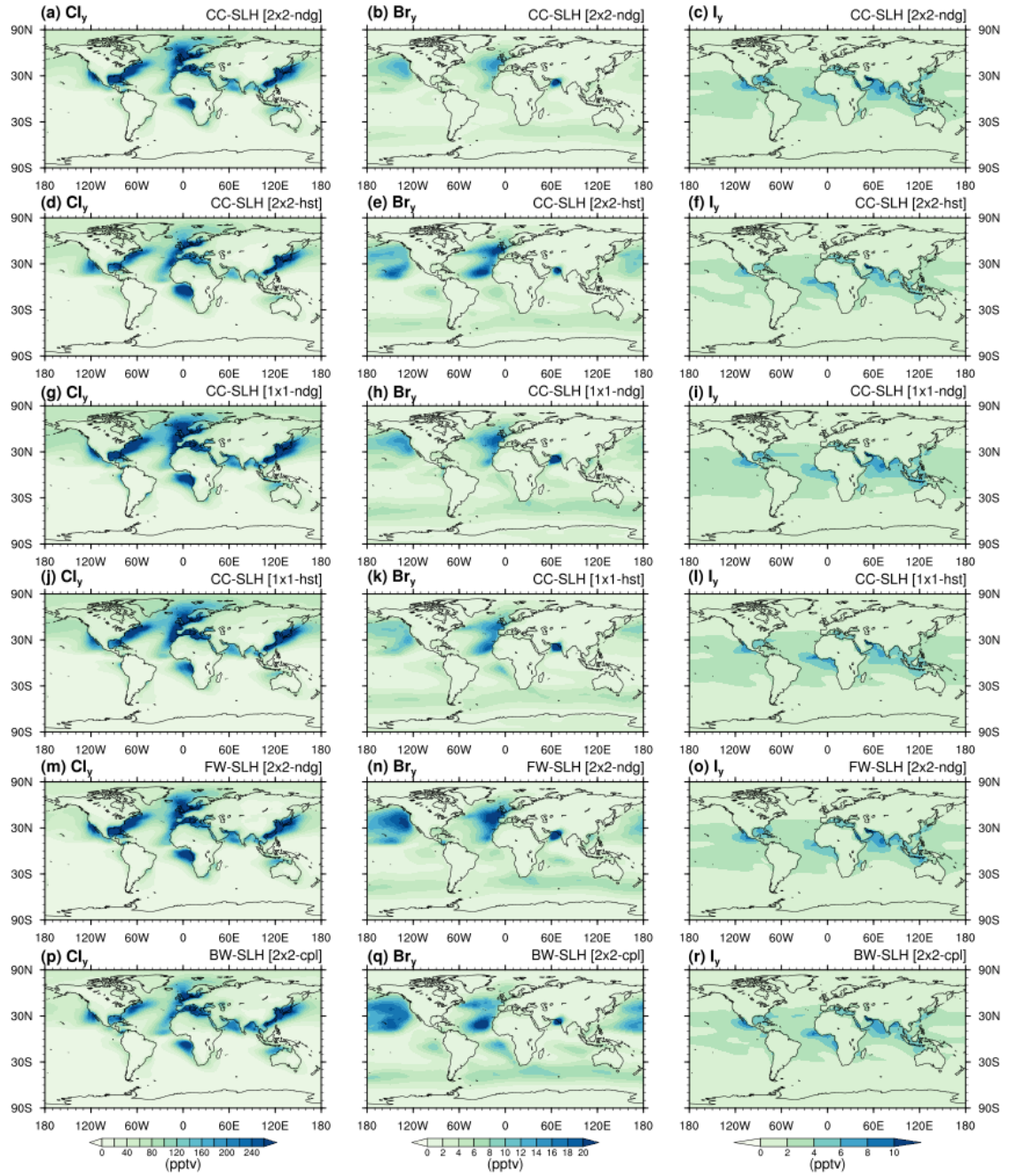


Figure S9: Comparison of the geographical distributions between different CSM2-SLH compsets and resolutions. Left, middle and right columns show the 2000-2005 annual mean distribution over the boundary layer for inorganic chlorine (Cl_y), bromine (Br_y) and iodine (I_y), respectively. (VSLC1). Each row presents results for individual CSM2-SLH experiments: CC-SLH [2x2-ndg] (1st row), CC-SLH [2x2-hst] (2nd row), CC-SLH [1x1-ndg] (3rd row), CC-SLH [1x1-hst] (4th row), FW-SLH [2x2-ndg] (5th row) and BW-SLH [2x2-cpl] (6th row).

Table S1: Photochemical Reactions separated by halogen family

Photolysis Reactions
$\text{CH}_2\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$
$\text{CHBr}_2\text{Cl} + h\nu \rightarrow 2^*\text{Br} + \text{Cl}$
$\text{CHBrCl}_2 + h\nu \rightarrow \text{Br} + 2^*\text{Cl}$
$\text{CH}_2\text{ICl} + h\nu \rightarrow \text{I} + \text{Cl}$
$\text{ICl} + h\nu \rightarrow \text{I} + \text{Cl}$
$\text{Cl}_2 + h\nu \rightarrow 2^*\text{Cl}$
$\text{ClO} + h\nu \rightarrow \text{Cl} + \text{O}$
$\text{OCIO} + h\nu \rightarrow \text{O} + \text{ClO}$
$\text{Cl}_2\text{O}_2 + h\nu \rightarrow 2^*\text{Cl}$
$\text{HOCl} + h\nu \rightarrow \text{OH} + \text{Cl}$
$\text{HCl} + h\nu \rightarrow \text{H} + \text{Cl}$
$\text{ClONO}_2 + h\nu \rightarrow \text{Cl} + \text{NO}_3$
$\text{ClONO}_2 + h\nu \rightarrow \text{ClO} + \text{NO}_2$
$\text{ClNO}_2 + h\nu \rightarrow \text{Cl} + \text{NO}_2$
$\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$
$\text{C}_2\text{Cl}_4 + h\nu \rightarrow 4^*\text{Cl}$
$\text{C}_2\text{H}_4\text{Cl}_2 + h\nu \rightarrow 2^*\text{Cl}$
$\text{CH}_2\text{Cl}_2 + h\nu \rightarrow 2^*\text{Cl}$
$\text{CH}_3\text{Cl} + h\nu \rightarrow \text{Cl} + \text{CH}_3\text{O}_2$
$\text{CHCl}_3 + h\nu \rightarrow \text{CHCl}_2\text{O}_2 + \text{Cl}$
$\text{COCl}_2 + h\nu \rightarrow 2^*\text{Cl} + \text{CO}$
$\text{COFCl} + h\nu \rightarrow \text{F} + \text{Cl}$
$\text{CCl}_4 + h\nu \rightarrow 4^*\text{Cl}$
$\text{CH}_3\text{CCl}_3 + h\nu \rightarrow 3^*\text{Cl}$
$\text{CFC11} + h\nu \rightarrow 3^*\text{Cl}$
$\text{CFC12} + h\nu \rightarrow 2^*\text{Cl}$
$\text{CFC113} + h\nu \rightarrow 3^*\text{Cl}$
$\text{HCFC22} + h\nu \rightarrow \text{Cl}$
$\text{CH}_3\text{Br} + h\nu \rightarrow \text{Br} + \text{CH}_3\text{O}_2$
$\text{CF}_3\text{Br} + h\nu \rightarrow \text{Br}$
$\text{CF}_2\text{ClBr} + h\nu \rightarrow \text{Br} + \text{Cl}$
$\text{CFC114} + h\nu \rightarrow 2^*\text{Cl}$
$\text{CFC115} + h\nu \rightarrow \text{Cl}$
$\text{HCFC141B} + h\nu \rightarrow 2^*\text{Cl}$
$\text{HCFC142B} + h\nu \rightarrow \text{Cl}$
$\text{IBr} + h\nu \rightarrow \text{I} + \text{Br}$
$\text{CH}_2\text{IBr} + h\nu \rightarrow \text{I} + \text{Br}$
$\text{CHBr}_3 + h\nu \rightarrow 3^*\text{Br}$
$\text{CH}_2\text{Br}_2 + h\nu \rightarrow 2^*\text{Br}$
$\text{BrO} + h\nu \rightarrow \text{Br} + \text{O}$
$\text{HOBr} + h\nu \rightarrow \text{Br} + \text{OH}$
$\text{HBr} + h\nu \rightarrow \text{Br} + \text{H}$
$\text{BrONO}_2 + h\nu \rightarrow \text{Br} + \text{NO}_3$
$\text{BrONO}_2 + h\nu \rightarrow \text{BrO} + \text{NO}_2$
$\text{BrNO}_2 + h\nu \rightarrow \text{Br} + \text{NO}_2$
$\text{BrNO}_2 + h\nu \rightarrow \text{BrO} + \text{NO}$
$\text{Br}_2 + h\nu \rightarrow 2^*\text{Br}$
$\text{H2402} + h\nu \rightarrow 2^*\text{Br}$
$\text{CH}_3\text{I} + h\nu \rightarrow \text{I} + \text{CH}_3\text{O}_2$
$\text{CH}_2\text{I}_2 + h\nu \rightarrow 2^*\text{I}$
$\text{I}_2 + h\nu \rightarrow 2^*\text{I}$
$\text{IO} + h\nu \rightarrow \text{I} + \text{O}$
$\text{OIO} + h\nu \rightarrow \text{I} + \text{O}_2$
$\text{INO} + h\nu \rightarrow \text{I} + \text{NO}$
$\text{INO}_2 + h\nu \rightarrow \text{I} + \text{NO}_2$
$\text{IONO}_2 + h\nu \rightarrow \text{I} + \text{NO}_3$
$\text{HOI} + h\nu \rightarrow \text{I} + \text{OH}$

$\text{HI} + h\nu \rightarrow \text{I} + \text{H}$
$\text{I}_2\text{O}_2 + h\nu \rightarrow \text{OIO} + \text{I}$
$\text{I}_2\text{O}_3 + h\nu \rightarrow \text{OIO} + \text{IO}$
$\text{I}_2\text{O}_4 + h\nu \rightarrow \text{OIO} + \text{OIO}$

Table S2: Arrhenius type Reactions separated by halogen family

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
$Br_2 + OH \rightarrow HOBr + Br$	$2.10 \times 10^{-11} e^{(240/T)}$
$Br + O_3 \rightarrow BrO + O_2$	$1.60 \times 10^{-11} e^{(-780/T)}$
$Br + HO_2 \rightarrow HBr + O_2$	$4.80 \times 10^{-12} e^{(-310/T)}$
$Br + CH_2O \rightarrow HBr + HO_2 + CO$	$1.70 \times 10^{-11} e^{(-800/T)}$
$BrO + BrO \rightarrow 2^*Br + O_2$	$1.50 \times 10^{-12} e^{(230/T)}$
$BrO + ClO \rightarrow Br + OCIO$	$9.50 \times 10^{-13} e^{(550/T)}$
$BrO + ClO \rightarrow Br + Cl + O_2$	$2.30 \times 10^{-12} e^{(260/T)}$
$BrO + ClO \rightarrow BrCl + O_2$	$4.10 \times 10^{-13} e^{(290/T)}$
$BrO + NO \rightarrow Br + NO_2$	$8.80 \times 10^{-12} e^{(260/T)}$

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

$\text{CH}_3\text{I} + \text{OH} \rightarrow \text{I} + \text{H}_2\text{O} + \text{HO}_2$	$2.90 \times 10^{-12} \text{e}^{(-1100/T)}$
$\text{CHBr}_2\text{Cl} + \text{OH} \rightarrow 2^*\text{Br} + \text{Cl}$	$9.00 \times 10^{-13} \text{e}^{(-420/T)}$
$\text{CHBr}_3 + \text{Cl} \rightarrow 3^*\text{Br} + \text{HCl}$	$4.85 \times 10^{-12} \text{e}^{(-850/T)}$
$\text{CHBr}_3 + \text{OH} \rightarrow 3^*\text{Br}$	$9.00 \times 10^{-13} \text{e}^{(-360/T)}$
$\text{CHBrCl}_2 + \text{OH} \rightarrow \text{Br} + 2^*\text{Cl}$	$9.40 \times 10^{-13} \text{e}^{(-510/T)}$
$\text{CHCl}_2\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow 2^*\text{Cl} + 2^*\text{HO}_2 + \text{CH}_2\text{O} + \text{CO}$	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.

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:
	$k_0 = 1.40 \times 10^{-28} \times (300/T)^{8.5}$
	$K_i = 4.0 \times 10^{-11} \times (300/T)^{1.2}$, $f=0.6$
$\text{C}_2\text{Cl}_4 + \text{Cl} + \text{M} \rightarrow \text{Cl} + \text{M}$	troe:
	$k_0 = 1.60 \times 10^{-29} \times (300/T)^{3.3}$
	$k_i = 3.1 \times 10^{-10} \times (300/T)^{1.0}$, $f=0.6$

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

Table S4: Global mean surface and tropospheric SLH loading for different experiments during present-day (2015–2020).

Experiment	Units ^{&}	CC-SLH [2×2-ndg]	CC-SLH [2×2-hst]	CC-SLH [1×1-ndg]	CC-SLH [1×1-hst]	FW-SLH [2×2-ndg]	BW-SLH [2×2-cpl]
Offline Sources							
VSL _{Cl}	Tropo (Gg yr ⁻¹)	1624.0	1658.8	1587.3	1603.7	1644.1	1652.9
VSL _{Br}	Tropo (Gg yr ⁻¹)	715.5	715.4	715.3	715.2	717.7	716.7
VSL _I	Tropo (Gg yr ⁻¹)	602.6	601.6	602.0	601.3	602.8	602.3
Online Sources							
Acid-displacement	Tropo (Gg yr ⁻¹)	20488.2	19036.5	20926.6	19212.2	20906.2	20936.3
SSA-dehal. Cl	Tropo (Gg yr ⁻¹)	3212.0	4051.7	4024.5	3730.4	4054.2	4686.6
SSA-dehal. Br	Tropo (Gg yr ⁻¹)	2323.7	3886.1	2961.4	2840.7	4224.9	5208.5
Oceanic Iodine	Surface (Gg yr ⁻¹)	2391.4	2189.0	2234.4	2143.6	2258.4	2321.3
Abundance							
VSL _{Cl}	Surface (pptv)	101.6	98.4	103.0	101.3	100.3	98.3
	Tropo (Gg)	419.1	415.2	437.2	433.6	413.0	418.6
VSL _{Br}	Surface (pptv)	8.5	7.9	8.6	8.2	8.4	7.7
	Tropo (Gg)	56.7	55.2	59.3	58.5	55.2	55.4
VSL _I	Surface (pptv)	1.2	1.1	1.2	1.1	1.2	1.0
	Tropo (Gg)	4.8	4.7	4.9	4.8	4.7	4.6
Cl _y	Surface (pptv)	37.4	36.0	40.8	37.5	38.3	36.8
	Tropo (Gg)	155.9	140.7	176.5	161.9	171.3	165.6
Br _y	Surface (pptv)	2.2	3.3	2.7	2.7	3.5	4.1
	Tropo (Gg)	19.8	19.8	22.7	20.9	20.5	22.1
I _y	Surface (pptv)	3.1	2.7	3.0	2.7	3.0	2.9
	Tropo (Gg)	17.3	16.8	15.3	15.5	16.0	15.7

[&]All tropospheric magnitudes have been computed considering the chemical tropopause ($O_3 < 150$ ppbv).

Table S5: Global mean surface and tropospheric changes in O₃, OH, and NO₂ abundance due to SLH during present-day (2015–2020).

Experiments	Units ^{&}	CC-SLH–CC-NOH [2×2-ndg]		CC-SLH–CC-NOH [2×2-hst]		CC-SLH–CC-NOH [1×1-ndg]		CC-SLH–CC-NOH [1×1-hst]		FW-SLH–FW-NOH [2×2-hst]		BW-SLH–BW-NOH [2×2-cpl]	
Atmos. Comp. [§]		Abs.	Perc.	Abs.	Perc.	Abs.	Perc.	Abs.	Perc.	Abs.	Perc.	Abs.	Perc.
ΔO_3	Surface (ppbv)	-6.2	-21.8	-7.0	-23.4	-8.1	-27.5	-8.5	-28.2	-6.3	-22.8	-7.7	-26.2
	Tropo (Gg)	-58.9	-18.0	-59.6	-18.3	-69.6	-21.3	-73.0	-22.1	-57.2	-17.7	-64.0	-19.6
ΔOH	Surface (ppqv)	-1.9	-3.0	-3.1	-4.6	-3.4	-5.4	-3.7	-5.7	-2.4	-3.7	-3.8	-5.7
	Tropo (Mg)	-13.0	-5.7	-14.6	-6.4	-20.8	-9.6	-21.0	-9.5	-14.8	-6.2	-15.3	-6.7
ΔNO_2	Surface (pptv)	-0.7	-0.1	-3.7	-0.6	1.0	0.2	-0.2	0.0	-4.8	-0.8	-5.2	-0.9
	Tropo (Gg)	-23.0	-6.5	-28.9	-8.3	-31.8	-8.9	-35.3	-9.7	-32.9	-0.9	-33.5	-9.5

[§]The absolute (Abs.) and percentage (Perc.) change in atmospheric abundance for each species is computed as (SLH – NOH) and [(SLH – NOH) / NOH] × 100%, respectively.

[&]All tropospheric magnitudes have been computed considering the chemical tropopause (O₃ < 150 ppbv).



Chart S1: Individual Fortran files and folders that have been updated within the CESM2-SLH CAM6-Chem structure. Blue font show files that have been modified, while green fonts highlight the new files and folders.

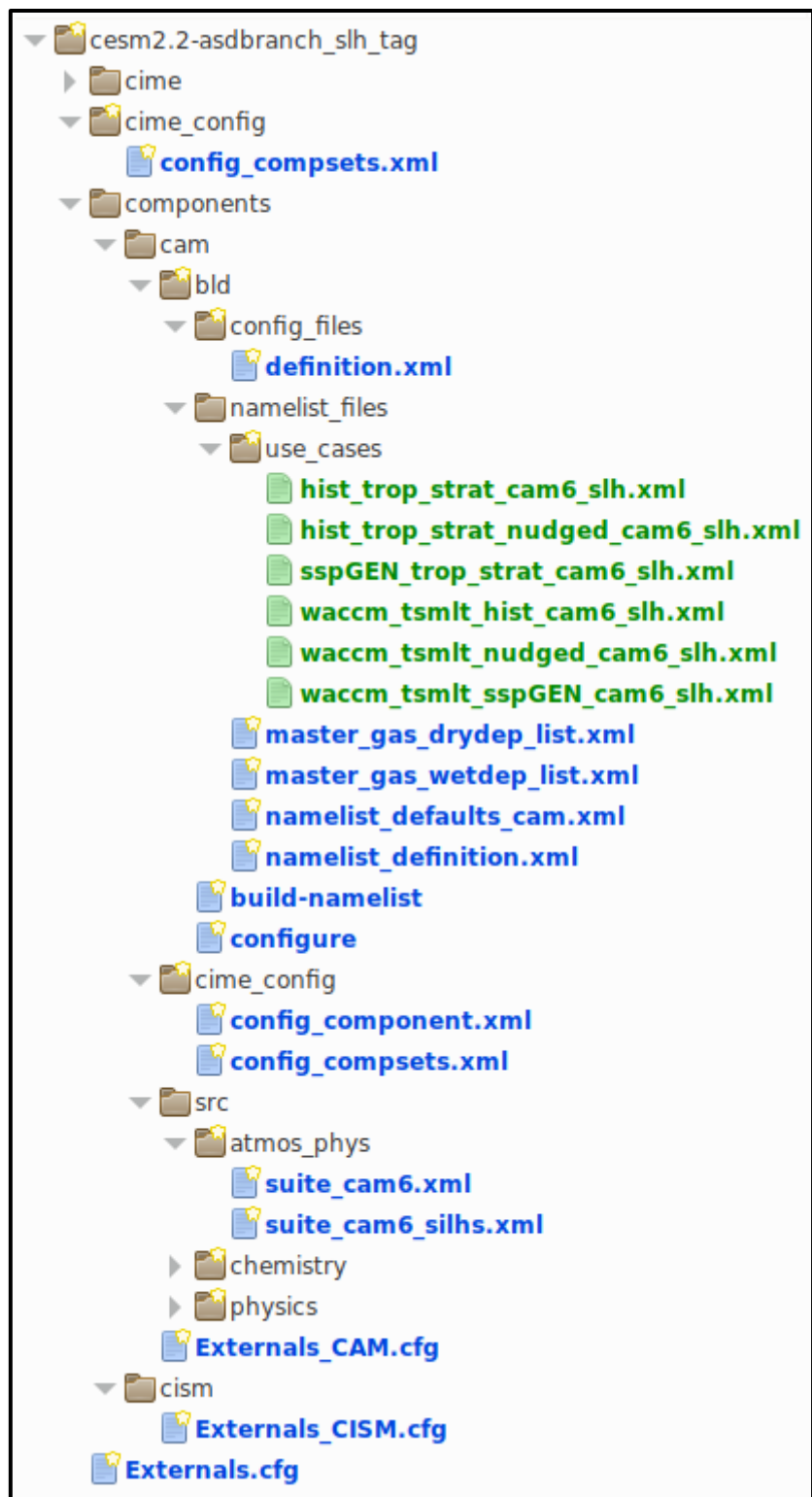


Chart S2: Individual configuration files and building scripts that have been updated within the CESM2-SLH CAM6-Chem structure. Blue font show files that have been modified, while green fonts highlight the new files and folders.

```

cam initfiles nl
ncdata = '$PATH/FC.f19 f19_mg17.L32.cesm2.2-asdbranch_slh_released.FCHIST_slh.Historical_SLH.cam.i.1980-01-01-00000.nc'
/
&chem_inparm
  srf_emis_specifier =
    'CHBR3 -> $PATH/emissions_CHBr3_chlorophyll_surface_Ordenez2012_flx1p15_cyclical_1850-2100_1.9x2.5_c240804.nc',
    'CH2BR2 -> $PATH/emissions_CH2Br2_chlorophyll_surface_Ordenez2012_flx1p15_cyclical_1850-2100_1.9x2.5_c240804.nc',
    'CH2BRCL -> $PATH/emissions_CH2BrCl_chlorophyll_surface_Ordenez2012_flx1p15_cyclical_1850-2100_1.9x2.5_c240804.nc',
    'CHBR2CL -> $PATH/emissions_CHBr2Cl_chlorophyll_surface_Ordenez2012_flx1p15_cyclical_1850-2100_1.9x2.5_c240804.nc',
    'CHBRCL2 -> $PATH/emissions_CHBrCl2_chlorophyll_surface_Ordenez2012_flx1p15_cyclical_1850-2100_1.9x2.5_c240804.nc',
    'CH3I -> $PATH/emissions_CH3I_chlorophyll_surface_Ordenez2012_cyclical_1850-2100_1.9x2.5_c240804.nc',
    'CH2I2 -> $PATH/emissions_CH2I2_chlorophyll_surface_Ordenez2012_cyclical_1850-2100_1.9x2.5_c240804.nc',
    'CH2IBR -> $PATH/emissions_CH2IBr_chlorophyll_surface_Ordenez2012_cyclical_1850-2100_1.9x2.5_c240804.nc',
    'CH2ICL -> $PATH/emissions_CH2ICl_chlorophyll_surface_Ordenez2012_cyclical_1850-2100_1.9x2.5_c240804.nc',
    'CH2CL2 -> $PATH/emissions_CH2CL2_NoNeg_surface_Claxton2020_flx1p15_serial_1850-2100_1.9x2.5_c240722.nc',
    'C2CL4 -> $PATH/emissions_C2CL4_NoNeg_surface_Claxton2020_flx1p15_serial_1850-2100_1.9x2.5_c240722.nc',
    'I2 -> $PATH/emissions_I2_ocean_surface_PradosRoman2015_online_1850-2100_1.9x2.5_c240804.nc',
    'HOI -> $PATH/emissions_HOI_ocean_surface_PradosRoman2015_online_1850-2100_1.9x2.5_c240804.nc'
  xs_long_file = '$PATH/temp_prs_GT200nm_c221005mm_slh.nc'
  xs_short_file = '$PATH/xs_short_c221005mm_slh.nc'
/
&chem_surfvals_nl
  flbc_file = '$PATH/LBC_1750-2100_CMIP6_0p5degLat_HIST_c170126_SSP370_c180905_VSL_Cl_CHCL3x1p15_C2H4CL2x1p15_c20240731.nc'
  flbc_list = 'CCL4', 'CF2CLBR', 'CF3BR', 'CFC11', 'CFC113', 'CFC12', 'CH3BR', 'CH3CCL3', 'CH3CL', 'CH4', 'CO2', 'H2',
    'HCFC22', 'N2O', 'CFC114', 'CFC115', 'HCFC141B', 'HCFC142B', 'H2402', 'OCS', 'SF6', 'CHCL3', 'C2H4CL2'
/
&wetdep_inparm
  gas_wetdep_ice_uptake_list = 'HN03', 'CLON02', 'HCL', 'HOCL', 'BRN02', 'CLN02', 'I202', 'I203', 'I204'
  gas_wetdep_list =
    'CLON02', 'HOCL', 'HCL', 'COFCL', 'BRON02', 'HOB', 'HBR', 'BRCL',
    'CLN02', 'BRN02', 'BR2',
    'ION02', 'INO2', 'HI', 'IO', 'OIO', 'ICL',
    'IBR', 'I202', 'I203', 'I204', 'CHCL202', 'COCL2'
/
&drydep_inparm
  drydep_list =
    'CLON02', 'HCL', 'HOCL', 'CLN02', 'BRON02', 'HBR', 'HOB', 'BRN02', 'BR2',
    'ION02', 'HI', 'HOI', 'INO2', 'I202', 'I203', 'I204', 'CHCL202', 'COCL2'
/
&slh_nl
  ssadehal_scalingfactor = 1.70D0
  ssahno3_scalingfactor = 1.00D0
  ssan2o5_scalingfactor = 1.00D0
  liqfraprx_scalingfactor_i = 1.00D0
  icefraprx_scalingfactor_i = 1.70D0
  icefraprx_scalingfactor_br = 2.00D0
/

```

Chart S3: User defined namelist variables and parameters that must be updated in `user_nl_cam` to properly configure CESM2-SLH compsets. Example changes for the free-running *FCHIST_slh* compset with coarse $2^\circ \times 2^\circ$ resolution. Blue shading shows files and or variables that have been modified, while green shading highlights the new `&slh_nl` scaling factors.