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Supplement of

Using a two-stage Rosenbrock solver to increase computational efficiency in the DOE's Exascale Earth System Model version 1 (E3SMv1)

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Table S1. The corresponding gas species and aerosols involved in the chemUCI, with the specified order after the matrix permutation. The formula and description are based on Lamarque et al. (2012) and Emmons et al. (2020).

Index	Species	Chemical Formula or Description
1	H2SO4	H2SO4, sulfuric acid
2	SOAG	SOA gas phase precursor
3	so4_a1	Sulfate aerosol, MAM accumulation mode
4	so4_a2	sulfate aerosol, MAM Aitken mode
5	so4_a3	sulfate aerosol, MAM coarse mode
6	pom_a1	primary organic matter, MAM accumulation mode
7	pom_a3	primary organic matter, MAM coarse mode
8	pom_a4	primary organic matter, MAM primary carbon mode
9	soa_a1	SOA, MAM accumulation mode
10	soa_a2	SOA, MAM Aitken mode
11	soa_a3	SOA, MAM coarse mode
12	bc_a1	black carbon, MAM accumulation mode
13	bc_a3	black carbon, MAM coarse mode
14	bc_a4	black carbon, MAM primary carbon mode
15	dst_a1	dust, MAM accumulation mode
16	dst_a3	dust, MAM coarse mode
17	ncl_a1	sea salt, MAM accumulation mode
18	ncl_a2	sea salt, MAM Aitken mode
19	ncl_a3	sea salt, MAM coarse mode
20	mom_a1	marine organic matter, MAM accumulation mode
21	mom_a2	marine organic carbon, MAM Aitken mode
22	mom_a3	marine organic matter, MAM coarse mode
23	mom_a4	marine organic carbon, MAM primary carbon mode
24	num_a1	aerosol number concentration, MAM accumulation mode
25	num_a2	aerosol number concentration, MAM Aitken mode
26	num_a3	aerosol number concentration, MAM coarse mode
27	num_a4	aerosol number concentration, MAM primary carbon mode
28	SO2	SO2, sulfur dioxide
29	H2O2	H2O2, hydrogen peroxide

30	PAN	CH3CO3NO2, peroxy acetyl nitrate
31	DMS	CH3SCH3, dimethyl sulfide
32	N2O5	N2O5, dinitrogen pentoxide
33	C2H4	C2H4, ethene
34	ISOP	C5H8, isoprene
35	HNO3	HNO3, nitric acid
36	HNO4	HNO4, peroxynitric acid
37	CH3OOH	CH3OOH, methyl hydroperoxide
38	C2H5OOH	C2H5OOH, ethyl hydroperoxide
39	CH2O	CH2O, formaldehyde
40	MVKO2	
41	ROHO2	
42	C2H5O2	C2H5O2, ethylperoxy radical
43	ISOPO2	HOCH2COOCH3CHCH2
44	MVKMACR	
45	CH3CHO	CH3CHO, acetaldehyde
46	CH3CO3	CH3CO3, acetylperoxy radical
47	NO	NO, nitric oxide
48	CH3O2	CH3O2, methylperoxy radical
49	NO2	NO2, nitrogen dioxide
50	HO2	HO2, hydroperoxyl radical
51	NO3	NO3, nitrate radical
52	OH	OH, hydroxyl radical
53	O3	O3, ozone

Table S2. The corresponding gas species and aerosols involved in the trop_strat_mozart_mam4, with the specified order after the matrix permutation. The formula and description are based on Lamarque et al. (2012) and Emmons et al. (2020).

Index	Species	Chemical Formula or Description
1	NH4	NH4+ ammonium ion aerosol
2	SOA	Secondary Organic Aerosols
3	H2SO4	H2SO4, sulfuric acid
4	SOAG	SOA gas phase precursor
5	so4_a1	Sulfate aerosol, MAM accumulation mode
6	pom_a1	primary organic matter, MAM accumulation mode
7	soa_a1	SOA, MAM accumulation mode
8	bc_a1	black carbon, MAM accumulation mode
9	dst_a1	dust, MAM accumulation mode
10	ncl_a1	sea salt, MAM accumulation mode
11	mom_a1	marine organic matter, MAM accumulation mode
12	num_a1	aerosol number concentration, MAM accumulation mode
13	so4_a2	sulfate aerosol, MAM Aitken mode
14	soa_a2	SOA, MAM Aitken mode
15	ncl_a2	sea salt, MAM Aitken mode
16	mom_a2	marine organic carbon, MAM Aitken mode
17	num_a2	aerosol number concentration, MAM Aitken mode
18	dst_a3	dust, MAM coarse mode
19	ncl_a3	sea salt, MAM coarse mode
20	so4_a3	sulfate aerosol, MAM coarse mode
21	bc_a3	black carbon, MAM coarse mode
22	pom_a3	primary organic matter, MAM coarse mode
23	soa_a3	SOA, MAM coarse mode
24	mom_a3	marine organic matter, MAM coarse mode
25	num_a3	aerosol number concentration, MAM coarse mode
26	pom_a4	primary organic matter, MAM primary carbon mode
27	bc_a4	black carbon, MAM primary carbon mode
28	mom_a4	marine organic carbon, MAM primary carbon mode
29	num_a4	aerosol number concentration, MAM primary carbon mode

30	BIGALK	C5H12, lumped alkanes C>3
31	BIGENE	C4H8, lumped alkanes C>3
32	NH3	NH3, ammonia
33	CH3CN	CH3CN, acetonitrile
34	CL2O2	CL2O2, chlorine monoxide dimer
35	C3H8	C3H8, propane
36	SO2	SO2, sulfur dioxide
37	TOLUENE	C7H8, toluene
38	CRESOL	C7H8O, lumped cresols (hydroxymethylbenzenes)
39	EOOH	HOCH2CH2OOH, hydroxyhydroperoxide from OH + ethene chmistry
40	OCLO	OClO, chlorine dioxide
41	C2H2	C2H2, ethyne (acetylene)
42	CL2	CL2, chlorine
43	XOH	C7H10O6
44	N	N, nitrogen atom
45	HCN	HCN, hydrogen cyanide
46	BRCL	BrCl, bromine chloride
47	DMS	CH3SCH3, dimethyl sulfide
48	C2H5OH	C2H5OH, ethanol
49	EO	HOCH2CH2O, hydroxyalkoxy radical from OH + ethene chemistry
50	C2H6	C2H6, ethane
51	N2O5	N2O5, dinitrogen pentoxide
52	ENEO2	C4H9O3, lumped hydroxyperoxy radical from OH + ethene chmistry
53	MEKOOH	C4H8O3, hydroperoxide from MEK oxidation
54	MACROOH	C4H8O4, peroxide from methacrolein
55	C2H5OOH	C2H5OOH, ethyl hydroperoxide
56	XOOH	C5H10O5, lumped hydroperoxide from XO2 chemistry
57	C2H4	C2H4, ethene
58	HYDRALD	C5H8O2, lumped unsaturated hydroxycarbonyl
59	TOLOOH	C7H10O5, bicyclic hydroperoxide from toluene
60	C3H7OOH	C3H7OOH, propyl hydroperoxide
61	ROOH	CH3COCH2OOH, acetone hydroperoxide

62	HCOOH	HCOOH, formic acid
63	HO2NO2	HO2NO2, pernitric acid
64	ONIT	CH3COCH2ONO2
65	CH3OOH	CH3OOH, methyl hydroperoxide
66	MEK	C4H8O, methyl ethyl ketone
67	HOCH2OO	HOCH2OO, formaldehyde/HO2 adduct
68	TERPOOH	C10H18O3, hydroxy hydroperoxide from terpene 0 double bonds
69	PAN	CH3CO3NO2, peroxy acetyl nitrate
70	CH3COOOH	CH3COOOH, peracetic acid
71	TOLO2	C7H9O5, bicyclic peroxy radical from toluene
72	BIGALD	C5H6O2, lumped aldehyde from terpene ozonolysis
73	CH3OH	CH3OH, methanol
74	ISOPOOH	C5H10O3, unsaturated hydroxyhydroperoxide
75	BRONO2	BrONO2, bromine nitrate
76	MPAN	CH2CCH3CO3NO2, methacryloyl peroxynitrate
77	POOH	C3H6OHOOH, propene-derived hydroxy hydroperoxide
78	EO2	HOCH2CH2O2, hydroxyperoxy radical from OH + ethene chemistry
79	CH3COOH	CH3COOH, acetic acid
80	C10H16	C10H16
81	H2O2	H2O2, hydrogen peroxide
82	ALKOOH	C5H12O2, lumped alkane hydroperoxide
83	MEKO2	C4H7O3, peroxy radical formed from MEK oxidation
84	GLYOXAL	C2H2O2, glyoxal
85	ALKO2	C5H11O2, lumped alkane peroxy radical from BIGALK
86	CH3COCH3	CH3COCH3, acetone
87	PO2	C3H6OHO2, propene-derived peroxy radical
88	HOBR	HOBr, hypobromous acid
89	C2H5O2	C2H5O2, ethylperoxy radical
90	GLYALD	HOCH2CHO, glycolaldehyde
91	HBR	HBr, hydrogen bromide
92	HNO3	HNO3, nitric acid
93	C3H7O2	C3H7O2, propylperoxy radical

94	ISOP	C5H8, isoprene
95	HOCL	HOCl, hypochlorous acid
96	CLONO2	ClONO2, chlorine nitrate
97	ONITR	C4H7NO4, lumped hydroxynitrates
98	TERPO2	C10H17O3, peroxy radical from terpenes+OH
99	C3H6	C3H6, propene
100	ISOPNO3	C5H8NO5, peroxy radical from isoprene NO3 oxidation
101	H2	H2, hydrogen
102	CO	CO, carbon monoxide
103	RO2	CH3COCH2O2, peroxy radical from acetone
104	HYAC	CH3COCH2OH, hydroxyacetone
105	CH3CHO	CH3CHO, acetaldehyde
106	MACR	CH2CCH3CHO, methacrolein
107	CH3COCHO	CH3COCHO, methyl glyoxal
108	XO2	C5H9O5, peroxy radical from ISOPOOH, IEPOX, HPALD
109	MVK	CH2CHCOCH3, methyl vinyl ketone
110	MACRO2	CH3COCHO2CH2OH, peroxy radical from OH addition to methacrolein
111	ISOPO2	HOCH2COOCH3CHCH2
112	MCO3	CH2CCH3CO3, peroxy radical from OH abstraction reaction with MACR
113	CH3CO3	CH3CO3, acetylperoxy radical
114	H2O	H2O
115	H	H, hydrogen atom
116	BRO	BrO, bromine monoxide
117	CH3O2	CH3O2, methylperoxy radical
118	CH2O	CH2O, formaldehyde
119	NO3	NO3, nitrate radical
120	O3	O3, ozone
121	HO2	HO2, hydroperoxyl radical
122	O	O, ground state atomic oxygen
123	NO2	NO2, nitrogen dioxide
124	CL	Cl, chlorine atom
125	NO	NO, nitric oxide

126	CLO	ClO, chlorine monoxide
127	BR	Br, bromine atom
128	OH	OH, hydroxyl radical
129	HCL	HCl, hydrogen chloride
130	O1D	O, excited state atomic oxygen (O1D)

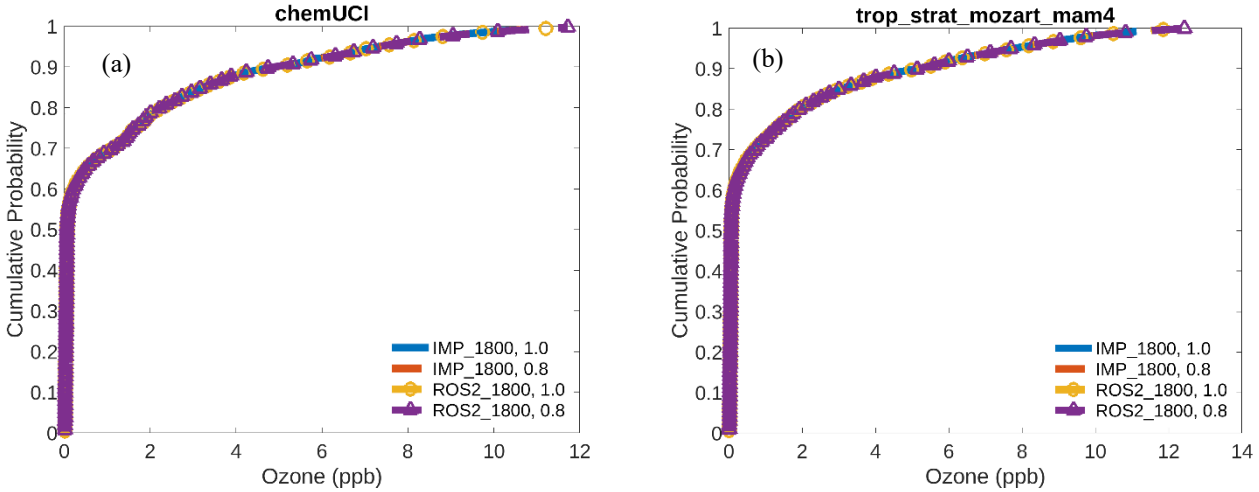
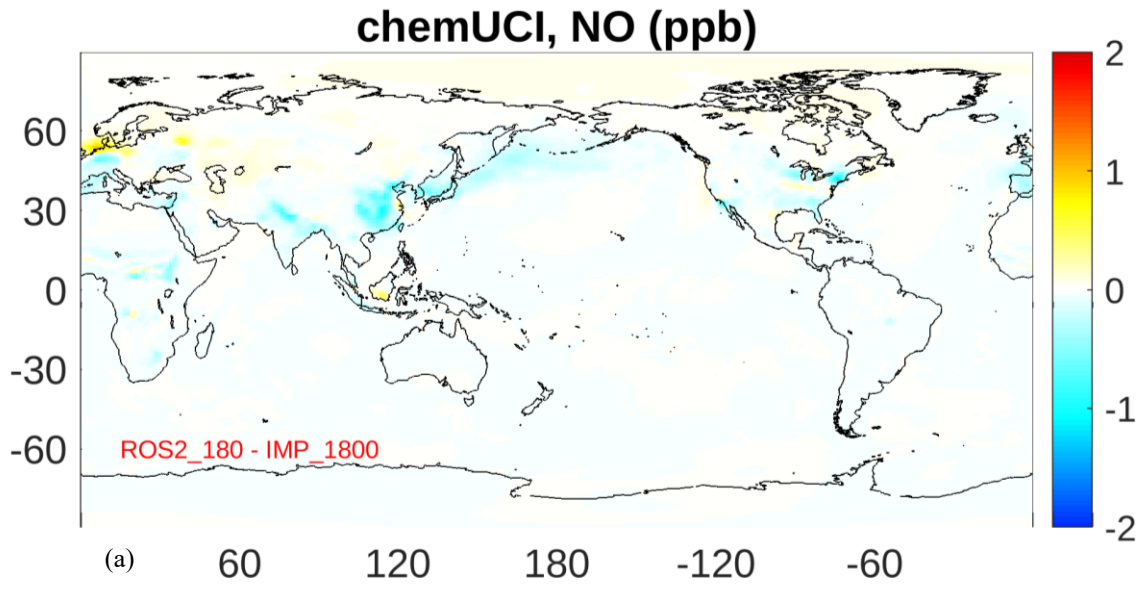


Figure S1. Empirical cumulative distribution function of box-model ozone for (a) chemUCI and (b) trop_strat_mozart_mam4 using the implicit solver (IMP) and the two-stage Rosenbrock solver (ROS2), under full external NOx emissions (1.0) and 80% of the external NOx emissions (0.8). The comparison is used to assess solver-to-solver consistency within each emissions scenario; the 100% and 80% cases are not expected to represent identical chemical states.



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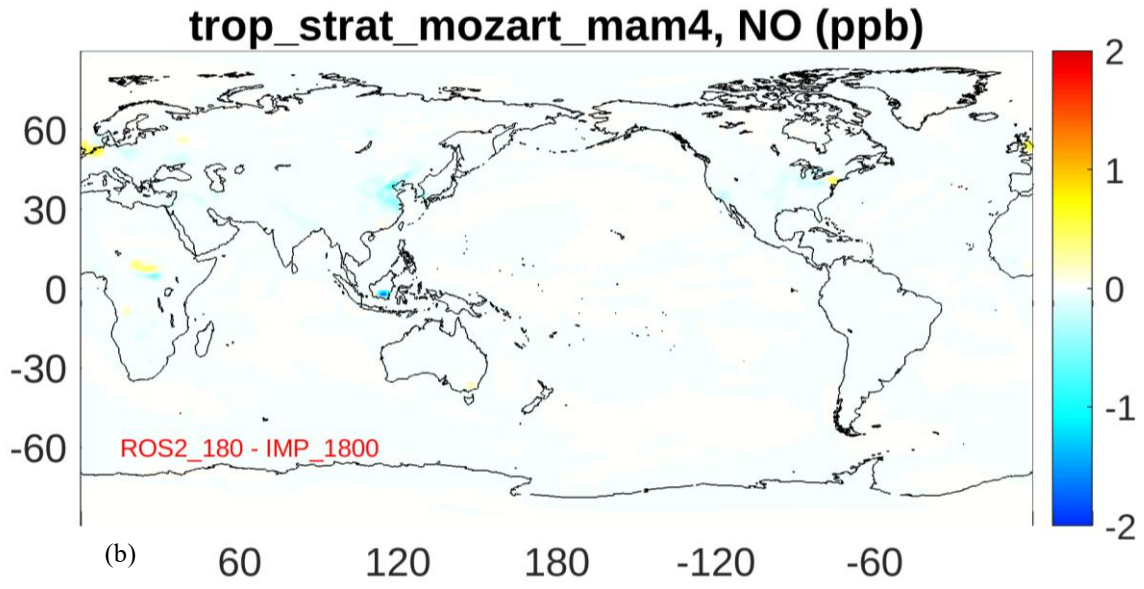

Figure S2. The global surface NO difference between ROS2_180 and IMP_1800 in (a) chemUCI and (b) trop_strat_mozart_mam4.

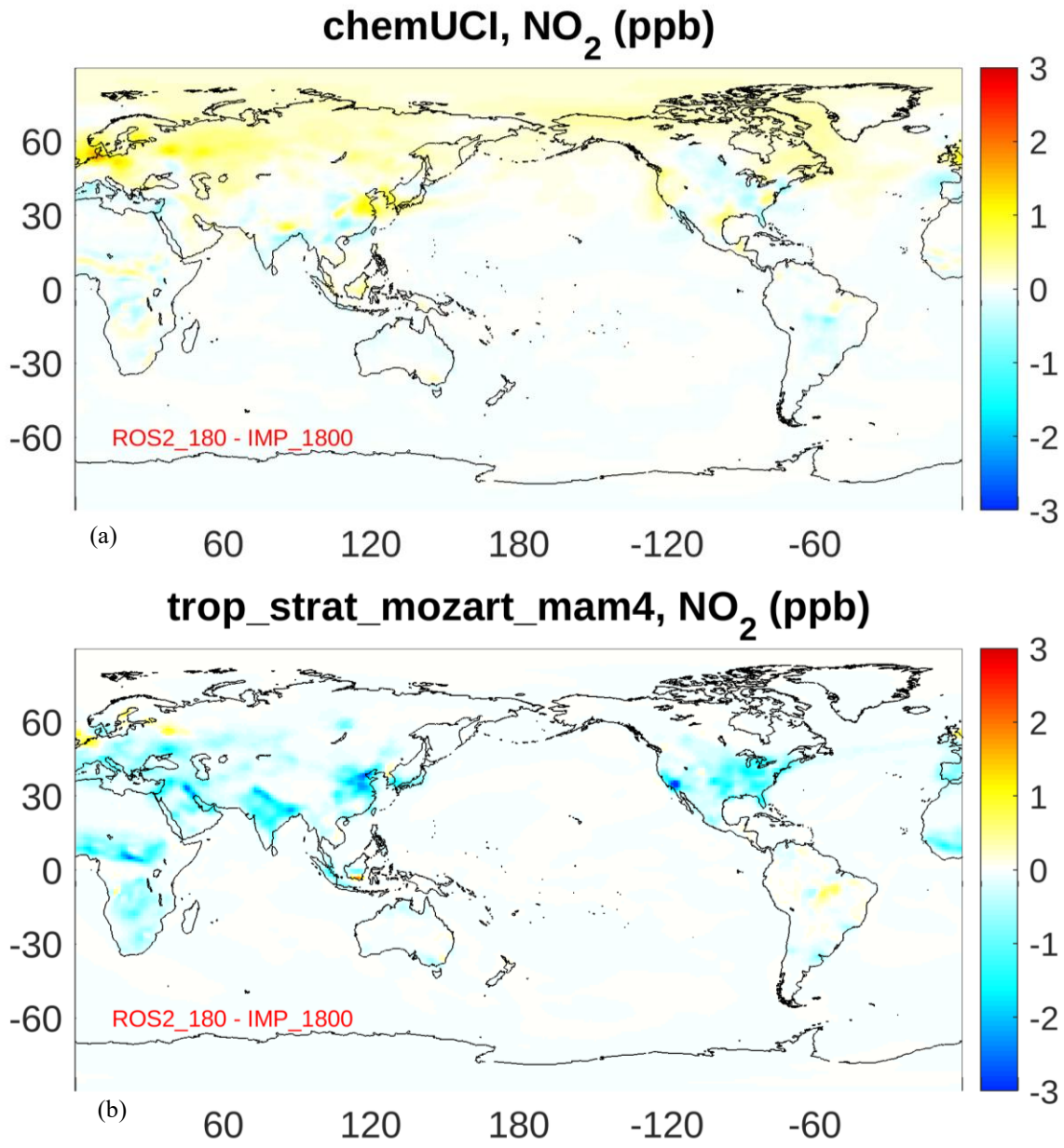

Figure S3. The global surface NO_2 difference between ROS2_180 and IMP_1800 in (a) chemUCI and (b) trop_strat_mozart_mam4.

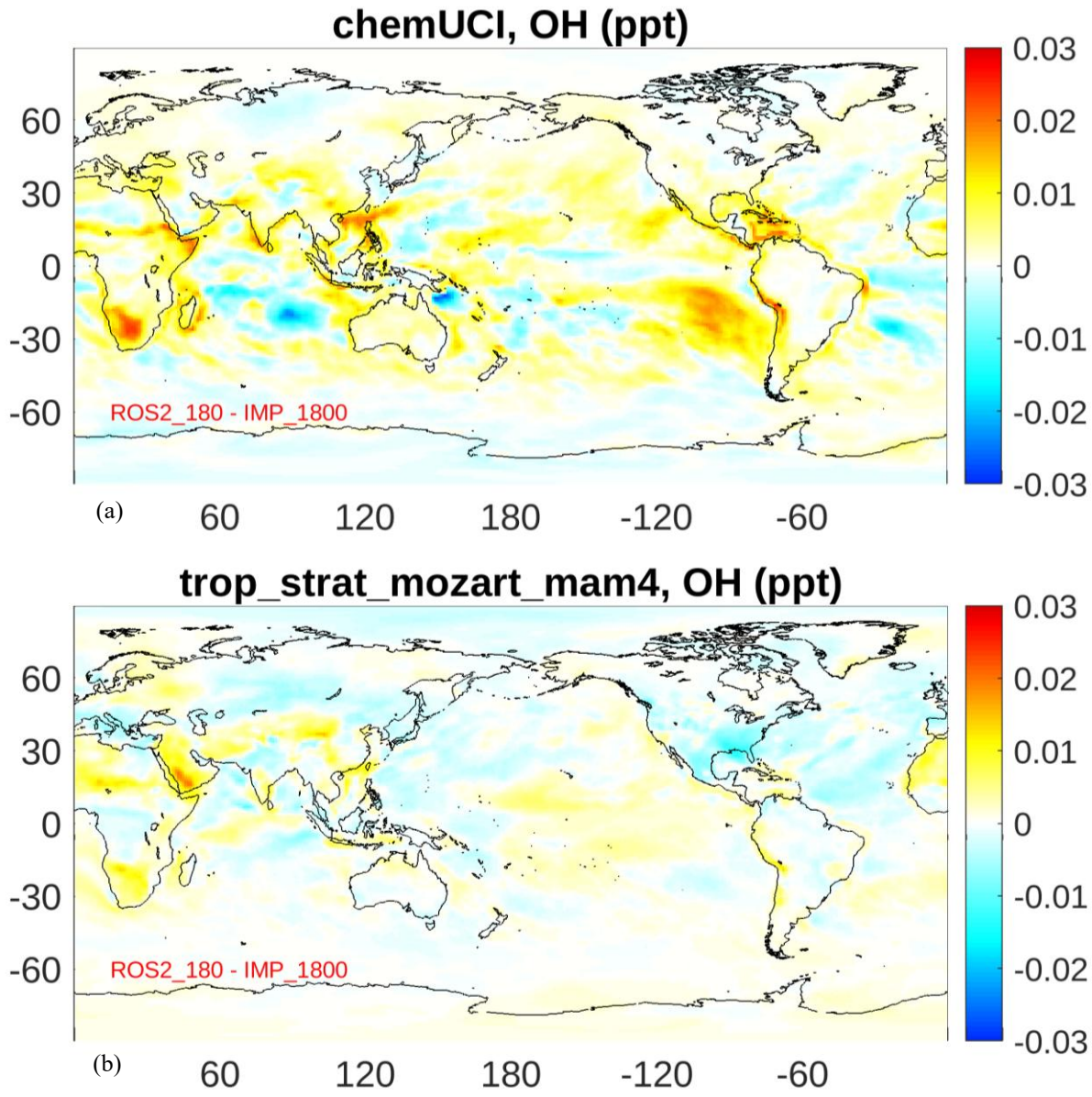

Figure S4. The global surface OH difference between ROS2_180 and IMP_1800 in (a) chemUCI and (b) trop_strat_mozart_mam4.

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