Description and evaluation of the UKCA stratosphere-troposphere chemistry scheme (StratTrop vn 1.0) implemented in UKESM1.

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Supplement

Table S1: List of experiments performed during the development of the StratTrop scheme. Each experiment was run for 20 years with the last 10 years analysed.

Experiment	Description	Production (Tg/yr)	Loss (Tg/yr)	Net (Tg/yr)	STE (inferred) (Tg)	τO_3 (days)	Burden O_3 (Tg)	τCH_4 (years)	Mean [OH] /10^5 cm^{-3}
A	Kinetics: 2005 Photolysis: FJx Emissions: Base ACCMIP Deposition: 2D	5650	4990	661	516 (489)	24.1	411	7.0	11.1

B	Kinetics: 2005; HO_2+NO->$HONO_2$ on. Photolysis: FJx Emissions: Base ACCMIP Deposition: 2D	4920	4410	505	558 (573)	25.3	386	8.0	9.43
C	Kinetics: 2011; HO_2+NO->$HONO_2$ on. Photolysis: FJx Emissions: Base ACCMIP Deposition: 2D	4920	4200	714	334 (299)	23.5	340	7.9	9.35
D	Kinetics: 2005; HO_2+NO->$HONO_2$ on. Photolysis: 2D Emissions: Base ACCMIP Deposition: 2D	3900	3250	649	387 (375)	28.9	343	11.7	6.07
E	Kinetics: 2011; HO_2+NO->$HONO_2$ on. Photolysis: FJx Emissions: Base ACCMIP Deposition: Wesley	4850	4200	653	349 (369)	22.8	330	7.7	9.56
F	Kinetics: 2011; HO_2+NO->$HONO_2$ on. Photolysis: FJx Emissions: Base ACCMIP + interactive CH_4 Deposition: Wesley	4630	4180	456	304 (513)	21.1	302	8.0	9.25
G	Kinetics: 2011; HO_2+NO->$HONO_2$ on. Photolysis: FJx Emissions: Base ACCMIP + Biogenic MeOH Deposition: Wesley	5000	4330	679	354 (363)	23.0	343	7.5	9.81

H	Kinetics: 2011; HO_2+NO->$HONO_2$ on. Photolysis: FJx Emissions: Base ACCMIP + Biogenic MeOH Deposition: Wesley Radiation: Non-interactive ozone.	5000	4360	634	412 (421)	23.0	347	7.5	9.81
I	Kinetics: 2011; HO_2+NO->$HONO_2$ on. Photolysis: FJx Emissions: Base ACCMIP + Biogenic MeOH Deposition: Wesley Chemistry: LLSF Isoprene (Squire et al., 2014)	4850	4140	708	351 (304)	23.2	333	7.77	9.52
J	Kinetics: 2011; HO_2+NO->$HONO_2$ on. Photolysis: FJx Emissions: Base ACCMIP + Biogenic MeOH Deposition: Wesley Chemistry: CheT2 Isoprene (Squire et al., 2014)	4830	4120	707	351 (305)	23.1	330	7.71	9.63
K	Kinetics: 2011; HO_2+NO->$HONO_2$ on. Photolysis: FJx Emissions: Base ACCMIP + Biogenic MeOH + 2*Isoprene Deposition: Wesley Chemistry: LLSF Isoprene (Squire et al., 2014)	5270	4560	718	337 (388)	22.5	350	8.65	8.39

L	Kinetics: 2011; HO_2+NO->$HONO_2$ on. Photolysis: FJx Emissions: Base ACCMIP + Biogenic MeOH + 0.5*Isoprene Deposition: Wesley Chemistry: LLSF Isoprene (Squire et al., 2014)	4470	3800	664	300 (336)	23.3	309	7.33	10.2
M	Kinetics: 2011; HO_2+NO->$HONO_2$ on. Photolysis: FJx Emissions: Base ACCMIP + Biogenic MeOH + 0.5*LNOx Deposition: Wesley	4460	3820	642	309 (332)	25.8	304	8.77	8.43
N	Kinetics: 2011; HO_2+NO->$HONO_2$ on. Photolysis: FJx Emissions: Base ACCMIP + Biogenic MeOH + 0.5*Soil NOx Deposition: Wesley	4860	4170	682	321 (353)	23.5	338	7.98	9.24
	ACCMIP mean	5230.0	4322.0	908.0		22.3	337±23	9.8±1.6	11.1±1.8

Key: FJx = Fast-JX photolysis; 2D = same photolysis scheme as used in HadGEM2-ES; Base ACCMIP = year 2000 emissions from Lamarque et al. (2010); Biogenic MeOH = climatology of biogenic MeOH emissions from Stavrakou et al. (2011); Deposition 2D = using the deposition scheme as described in Morgenstern et al. (2009); Deposition Wesley = using the Wesley deposition scheme discussed here; Chemistry LLSF isoprene = using the LLSF isoprene chemical mechanism as discussed in Squire et al. (2015); Chemistry CheT2 isoprene = using the CheT2 isoprene chemical mechanism as discussed in Squire et al. (2015);

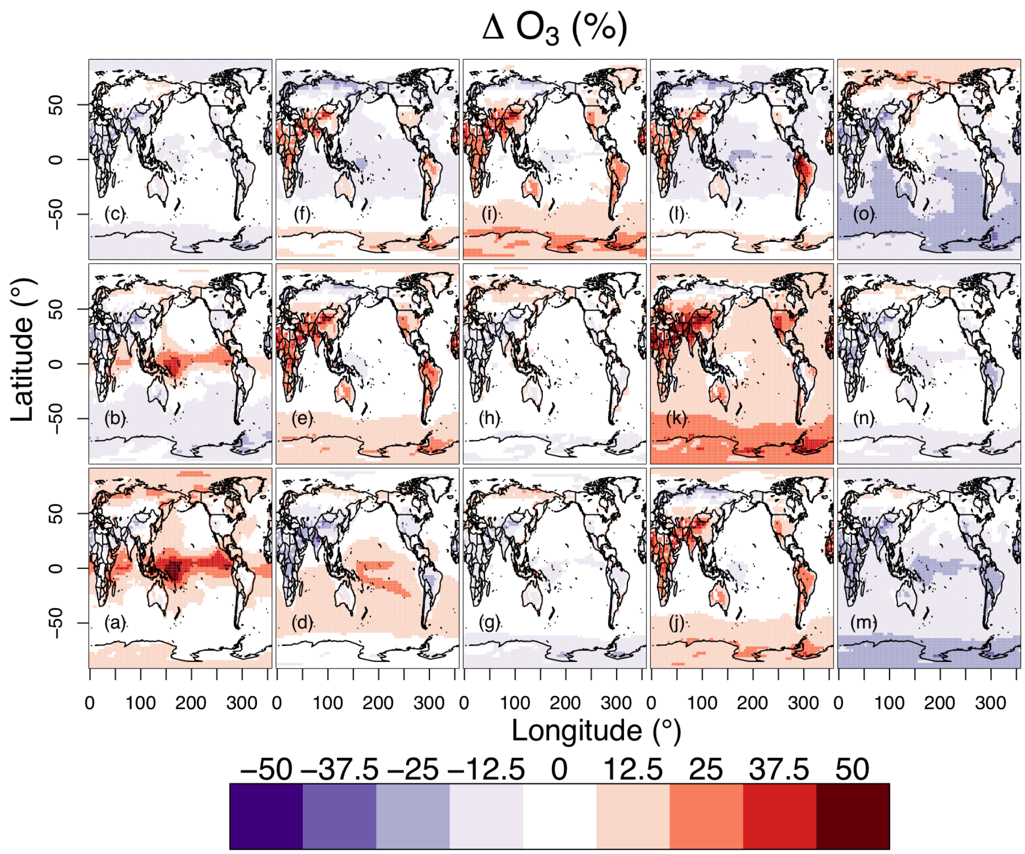

Figure S1: Comparison of changes in annual average surface ozone across the model simulations outlined in Table S1. Each model simulation was combined to generate an ensemble mean and the panels show the relative % difference {%((simulation$_i$-ensemble mean)/ensemble mean)} for each simulation to the ensemble mean.

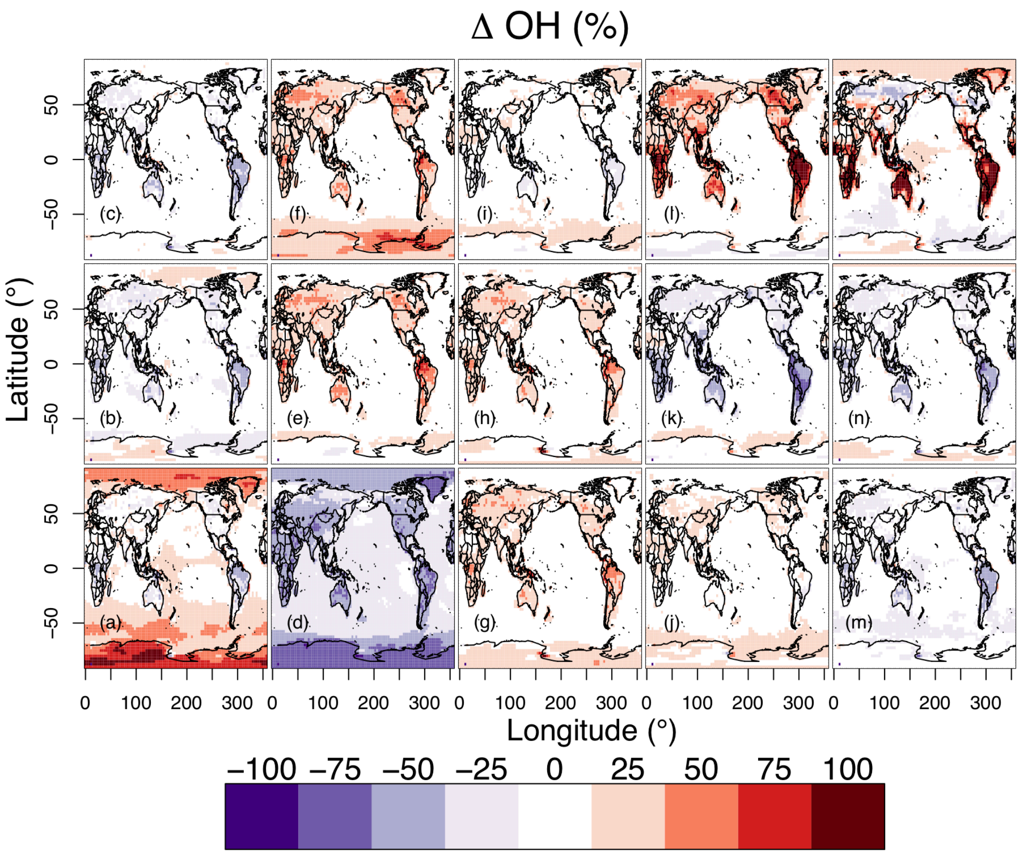

Figure S2: Comparison of changes in annual average surface hydroxyl radical across the model simulations outlined in Table S1. Each model simulation was combined to generate an ensemble mean and the panels show the relative % difference {%((simulation$_i$-ensemble mean)/ensemble mean)} for each simulation to the ensemble mean.

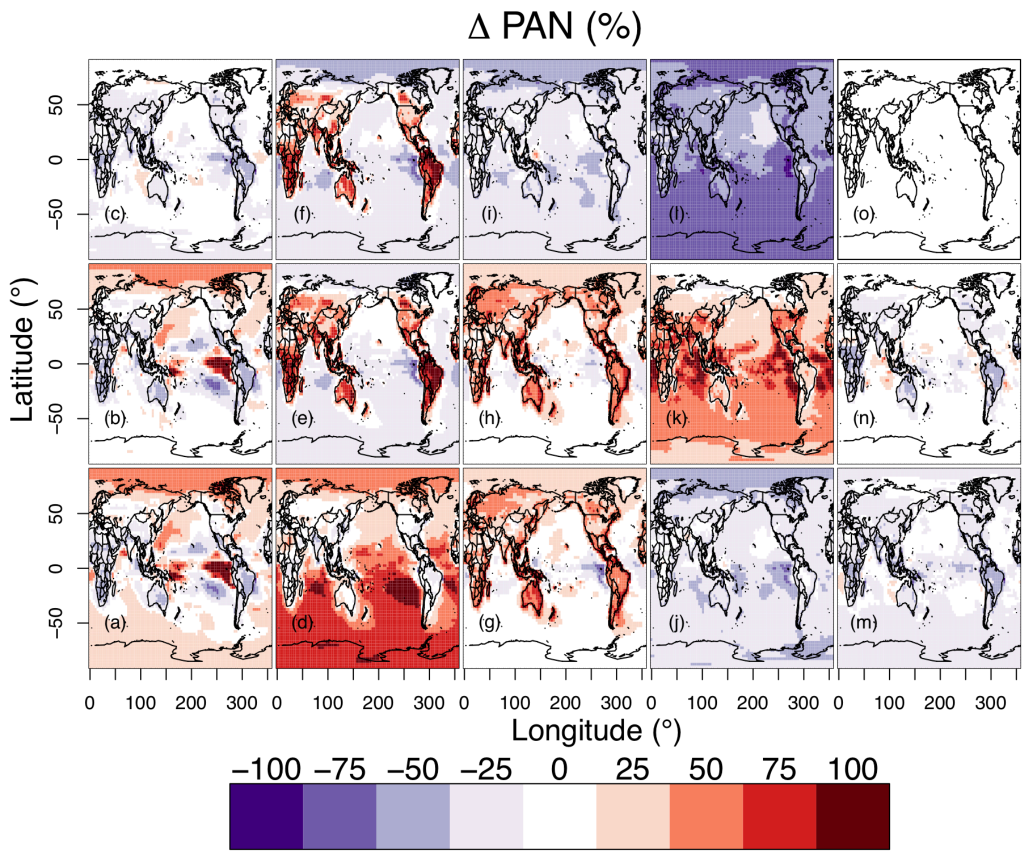

Figure S3: Comparison of changes in annual average surface PAN across the model simulations outlined in Table S1. Each model simulation was combined to generate an ensemble mean and the panels show the relative % difference {%((simulation$_i$-ensemble mean)/ensemble mean)} for each simulation to the ensemble mean.

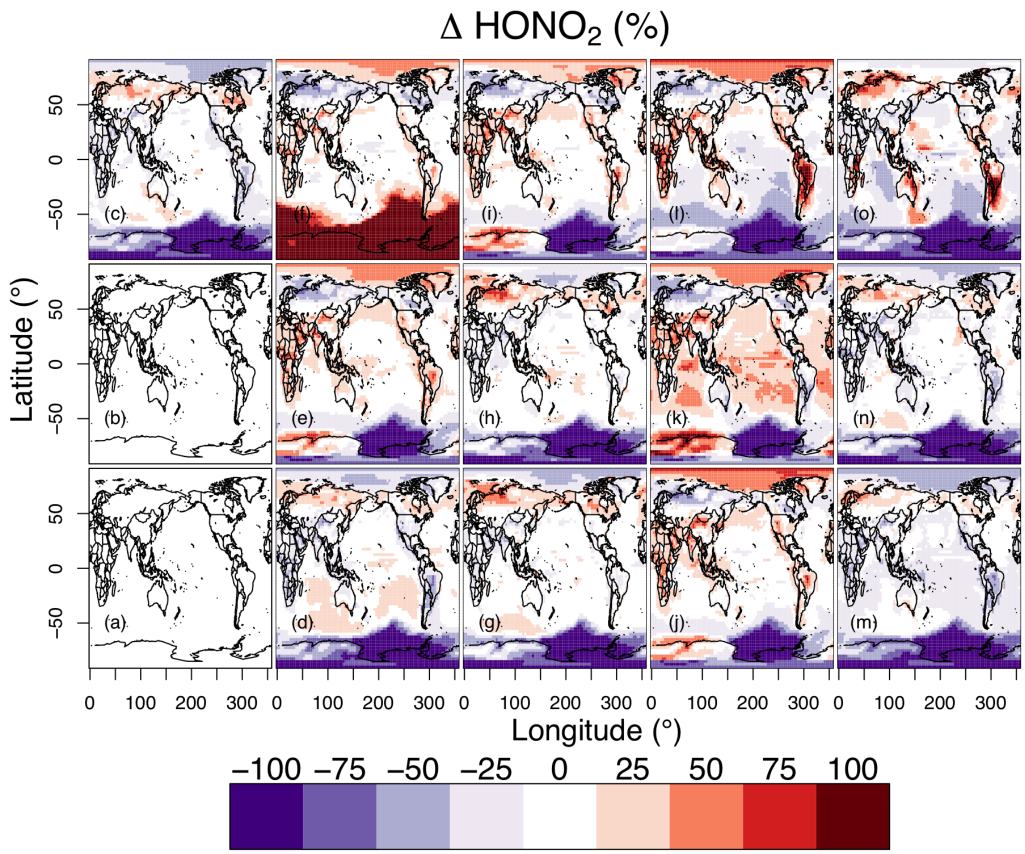

Figure S4: Comparison of changes in annual average surface nitric acid across the model simulations outlined in Table S1. Each model simulation was combined to generate an ensemble mean and the panels show the relative % difference {%((simulation$_i$-ensemble mean)/ensemble mean)} for each simulation to the ensemble mean.

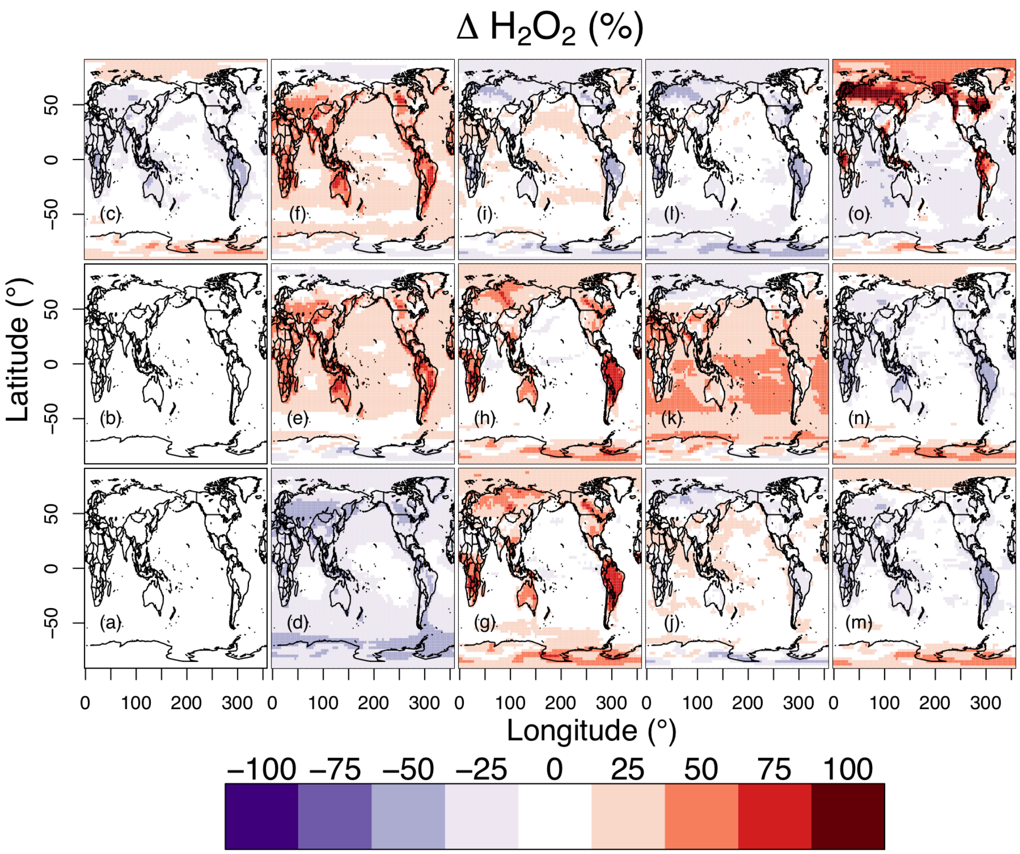

Figure S5: Comparison of changes in annual average surface hydrogen peroxide across the model simulations outlined in Table S1. Each model simulation was combined to generate an ensemble mean and the panels show the relative % difference {%((simulation$_i$-ensemble mean)/ensemble mean)} for each simulation to the ensemble mean.

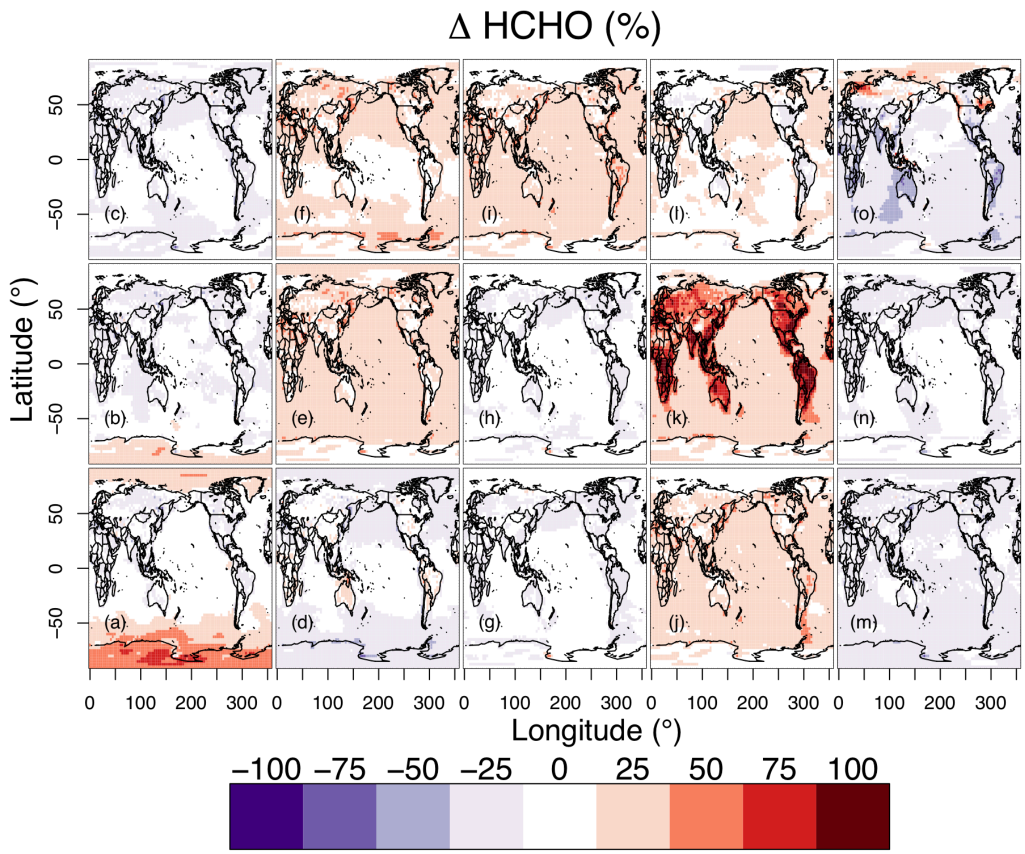

Figure S6: Comparison of changes in annual average surface formaldehyde across the model simulations outlined in Table S1. Each model simulation was combined to generate an ensemble mean and the panels show the relative % difference {%((simulation$_i$-ensemble mean)/ensemble mean)} for each simulation to the ensemble mean.

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