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Supplement of

Historical and future changes in air pollutants from CMIP6 models

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Table S1 – Brief description of the chemistry and aerosol set up within CMIP6 models used in this study

CMIP6 Model	Horiz. Res.	Vert levels (top level)	Aerosol scheme	Aerosol Species	Natural Sources	Treatment of SOA	Chemistry Scheme	Chemistry reactions	BVOCs	Model Ref
BCC-ESM1	2.813° x 2.813°	L26 (2.914 hPa)	Mass-based aerosol scheme. Prescribed stratospheric aerosols.	SO ₄ , BC (hydrophilic and hydrophobic), OM (hydrophilic and hydrophobic), sea salt (4 size bins), dust (4 size bins). No nucleation or coagulation of aerosols	Prescribed DMS seawater concentrations with emissions dependent on wind speed. Online emissions of sea-salt and dust aerosols. NO _x calculated from lightning.	Hydrophilic OC from anthropogenic emissions but also from natural sources calculated using a fixed yield, assumed to be equal to 10% of monoterpene emissions (from land surface model)	CAM-Chem (based on MOZART). Tropospheric only chemistry.	66 gas-phase chemical species with 33 photolytic reactions and 135 kinetic reactions.	Online biogenic emissions from dynamically evolving vegetation computed in the land model BCC-AVIM2.0 following the algorithm of MEGANv2.1 which has a dependence on light and temperature but also inhibits isoprene emissions based on CO ₂ .	(Wu et al., 2020)
CESM2-WACCM	0.9° x 1.25°	L70 (6x10 ⁻⁶ hPa)	MAM4 (modal scheme, simulating mass and number concentrations) with VBS-SOA	SO ₄ , BC, OM (both primary and secondary), sea salt, dust	Prescribed climatology of DMS seawater concentrations and emissions. Online emissions of sea-salt and dust aerosols. NO _x calculated from lightning. Soil NO _x and ocean CO, VOCs from POET	Explicit calculation of SOA using volatility basis set (VBS) where aromatic species, terpenes and isoprene are oxidised to produce a range of gas-phase SOA precursors with different volatilities. Formation of SOA linked to BVOCs emissions from interactive land surface scheme.	MOZART-TSMLT1 covering troposphere, stratosphere, mesosphere and lower thermosphere	231 gas-phase species, 150 photolytic reactions, 403 kinetic reactions and 30 heterogeneous reactions involving ClO _x , BrO _x , NO _x -HO _x -O _x , CO, CH ₄ and NMVOCs.	Online biogenic emissions (isoprene, monoterpenes, acetone, methanol, and other short and long-chained hydrocarbons) from dynamically evolving vegetation computed in the Community Land Model (CLM) using the MEGAN2.1 algorithm, which has dependence on light and temperature but also inhibits isoprene emissions based on CO ₂ .	(Gettelman et al., 2019; Tilmes et al., 2019; Emmons et al., 2020)
CNRM-ESM2-1	1.4° x 1.4°	L91 (80km)	TACTIC_v2. Tropospheric aerosols. Mass based aerosol scheme.	SO ₄ , BC (hydrophilic and hydrophobic), OM (hydrophilic and hydrophobic), sea salt (3 size bins), dust (3 size bins)	Prescribed DMS seawater concentrations. Online emissions of sea-salt and dust aerosols	Prescribed SOA from monthly inventory	No representation of lower tropospheric chemistry so not considered here.	N/A	N/A	(Michou et al., 2019; Séférian et al., 2019)
GFDL-ESM4	cubed-sphere (c96) grid, with ~100 km native resolution, regridded to 1.0° x 1.25°	L49 (0.01 hPa)	Bulk mass-based scheme. 5 size bins are used for sea salt and dust.	NH ₄ , SO ₄ , NO ₃ , NH ₄ , BC, OM, sea salt, dust	DMS and sea salt emissions calculated online as a function of wind speed (and a prescribed DMS seawater climatology). Dust emissions coupled to interactive vegetation. Lightning NO _x calculated online as a function of convection. Natural emissions of NO _x , CO, NMVOCs, H ₂ , and NH ₃ from POET. NH ₃ from seabird colonies. Two-way exchange of NH ₃ with ocean.	SOA formed simulated using an anthropogenic source from oxidation of C ₄ H ₁₀ tracer and a tracer representing BVOC emissions from vegetation	Interactive stratosphere-troposphere	43 photolysis reactions, 190 gas-phase kinetic reactions and 15 heterogeneous reactions. NO _x -HO _x -O _x - chemical cycles and CO, CH ₄ and NMVOC oxidation reactions	Online emissions of BVOCs (isoprene and monoterpenes) calculated from a prescribed vegetation cover using MEGAN2.1 algorithm, which has dependence on light and temperature but also inhibits isoprene emissions based on CO ₂ .	(Horowitz et al., 2019; Dunne et al., 2020)

GISS-E2-1-G	2° x 2.5°	L40 (0.1 hPa)	OMA (one moment aerosol scheme – mass based)	SO ₄ , NO ₃ , NH ₄ , BC, OM treated as externally mixed with prescribed and constant size distribution. Sea salt has two size classes. Sectional scheme for dust with 5 size bins that can be coated with SO ₄ and NO ₃ to increase solubility.	Sea salt, DMS, isoprene and dust emission fluxes are calculated interactively. Online NO _x calculated from lightning. Soil NO _x , ocean CO, VOCs from GEIA. NH ₃ from oceans. SO ₂ from volcanoes as in AeroCom.	Two-product model approximation to represent SOA formation from the oxidation of biogenic VOCs, including NO _x dependent chemistry yields.	Coupled troposphere-stratosphere chemistry scheme. Modified Carbon Bond Mechanism 4 (CBM-4) chemical mechanism	inorganic chemistry of O _x , NO _x , HO _x , CO, and organic chemistry of CH ₄ and lumped higher hydrocarbons (only isoprene and terpenes are explicitly taken into account), along with Cl and Br stratospheric chemistry and heterogenous reactions on PSCs and SO ₄ aerosols.	Emissions of isoprene from dynamically evolving vegetation are calculated interactively using the algorithm of Guenther et al., (1995), which has dependence on light and temperature. Terpene emissions are prescribed.	(Bauer et al., 2020)
HadGEM3-GC31-LL	1.25° x 1.875°	L85 (85km)	GLOMAP-Mode. (Modal scheme, mass and number). Mass based bin scheme used for dust.	SO ₄ , BC, OM, sea salt in 5 log-normal modes and dust in 6 bins	Prescribed climatologies of DMS seawater concentrations and BVOC emissions. No marine source of primary organics. Online emissions of sea-salt and dust aerosols	Fixed yield of SOA of 26% calculated from gas-phase oxidation reactions involving prescribed land-based monoterpene sources	Simplified sulphur chemistry for use with aerosol scheme	Oxidation for SO ₄ and simplified oxidation scheme (monoterpenes) for SOA	N/A	(Mulcahy et al., 2020)
MIROC6-ES2L	2.813° x 2.813°	L40 (3.0 hPa)	SPRINTAS.	SO ₄ , BC, OM, sea salt and dust in log-normal size distributions. External mixing assumed for SO ₄ , sea salt and dust aerosols.	Online emissions of DMS, sea-salt and dust aerosols. Primary marine organic aerosol emissions coupled to ocean biogeochemistry.	Prescribed emissions of isoprene and terpenes from GEIA used to convert to secondary organic carbon.	Simplified chemistry for use with aerosol scheme	Oxidation for SO ₄ and simplified oxidation scheme (isoprene and monoterpenes) for SOA	Prescribed emissions of isoprene and terpenes from GEIA.	(Takemura, 2012; Hajima et al., 2020)
MPI-ESM1.2-HAM	1.875° x 1.875°	L47 (0.01 hPa)	HAM2.3 (Modal scheme, mass and number)	SO ₄ , BC, OM, sea salt, dust in 7 log-normal modes	Interactive online emissions of DMS (using prescribed sea water concentrations), sea-salt and dust aerosols dependent on meteorology.	15% of natural terpene emissions at the surface (prescribed) form SOA. SOA have identical properties to primary organic aerosols	Simplified sulphur chemistry. Other fields prescribed.	Reactions involving SO ₂ , DMS and SO ₄ , including aqueous phase.	N/A	(Tegen et al., 2019)
MRI-ESM2-0	MRI-AGCM3.5: 1.125° x 1.125°, MASINGAR mk-2r4c: 1.875° x 1.875°, MRI-CCM2.1: 2.813° x 2.813°	L80 (0.01 hPa)	MASINGAR mk-2r4c	Mass-based scheme with externally mixed size distributions. SO ₄ (three categories), BC (hydrophilic and hydrophobic), OM (hydrophilic and hydrophobic), sea salt (10 size bins), dust (10 size bins).	Interactive online emissions of DMS (using prescribed Climatological DMS sea water concentrations), sea-salt, and dust aerosols dependent on meteorology. Online NO _x calculated from lightning. Climatological soil NO _x and ocean CO, VOCs emissions.	No explicit calculation: 14% of prescribed monoterpene and 1.68 % of isoprene emissions are assumed to form SOA.	Chemistry Climate Model version 2.1 (MRI-CCM2.1) covering troposphere, stratosphere, and mesosphere	90 chemical species and 259 chemical reactions (184 gas-phase reactions, 59 photolysis reactions, and 16 heterogeneous reactions) involving HO _x -NO _x -CH ₄ -CO cycles and NMVOC oxidation reactions, and halogen chemistry (Cl and Br)	Climatological BVOCs emissions	(Deushi and Shibata, 2011; Yukimoto et al., 2019)
NorESM2-LM	1.9° x 2.5°	L32 (3.64 hPa)	OsloAero6	SO ₄ , BC, OM, sea salt, dust. (log-normal modes)	Interactive emissions for sea-salt, biogenic primary OM (including MSA) and DMS over oceans, and interactive mineral dust and BVOC over land	Fixed SOA formation yields of 15% and 5% from oxidation of monoterpenes and isoprene	Simplified chemistry for use in aerosol scheme. Other fields prescribed.	Oxidation for SO ₄ and simplified oxidation scheme (isoprene and monoterpenes) for SOA	Online biogenic emissions from dynamically evolving vegetation computed in the Community Land Model (CLM) using the MEGAN2.1 algorithm, which has dependence on light and temperature but also inhibits isoprene emissions based on CO ₂ .	(Kirkevåg et al., 2018; Seland et al., 2020)

UKESM1-0-LL	1.25° x 1.875°	L85 (85km)	GLOMAP-Mode. (Modal scheme, mass and number). Mass based bin scheme used for dust.	SO ₄ , BC, OM, sea salt in 5 log-normal modes and dust in 6 bins	Dynamic vegetation and interactive ocean biogeochemistry used for online emissions of DMS, sea-salt and dust aerosols, as well as emissions of primary marine organics and biogenic organic compounds. Online NO _x calculated from lightning, soil NO _x and ocean CO, VOCs from POET	Fixed SOA yield of 26% from gas-phase oxidation reactions involving interactive land-based monoterpene sources.	UKCA coupled stratosphere-troposphere. Interactive photolysis	84 chemical tracers. Simulates chemical cycles of Ox, HOx and NO _x , as well as oxidation reactions of CO, CH ₄ and NMVOCs. In addition, heterogeneous processes, Cl and Br chemistry are included.	Dynamic vegetation and land surface model used to calculate interactive emissions of Isoprene and monoterpenes using light and temperature, but isoprene emissions are inhibited based on CO ₂ . Isoprene emissions coupled to chemistry and affect tropospheric O ₃ and methane lifetime. Monoterpenes only affect SOA.	(Archibald et al., 2020; Mulcahy et al., 2020)
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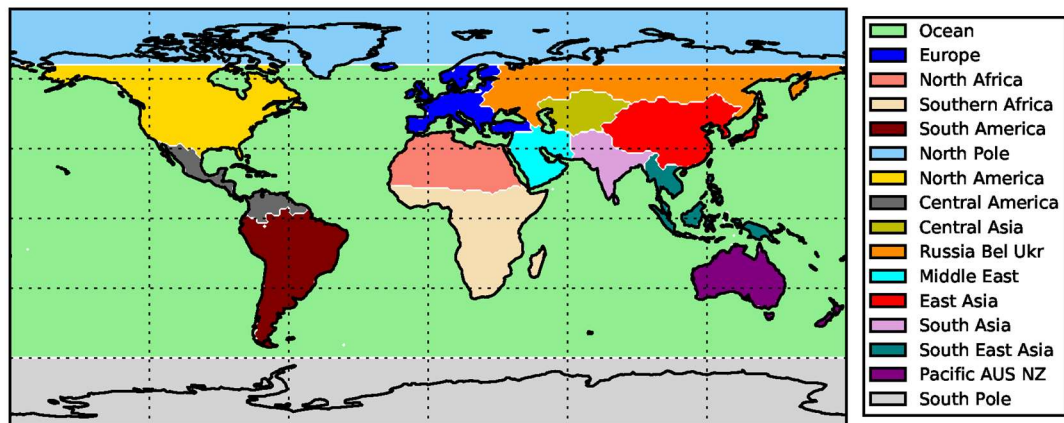
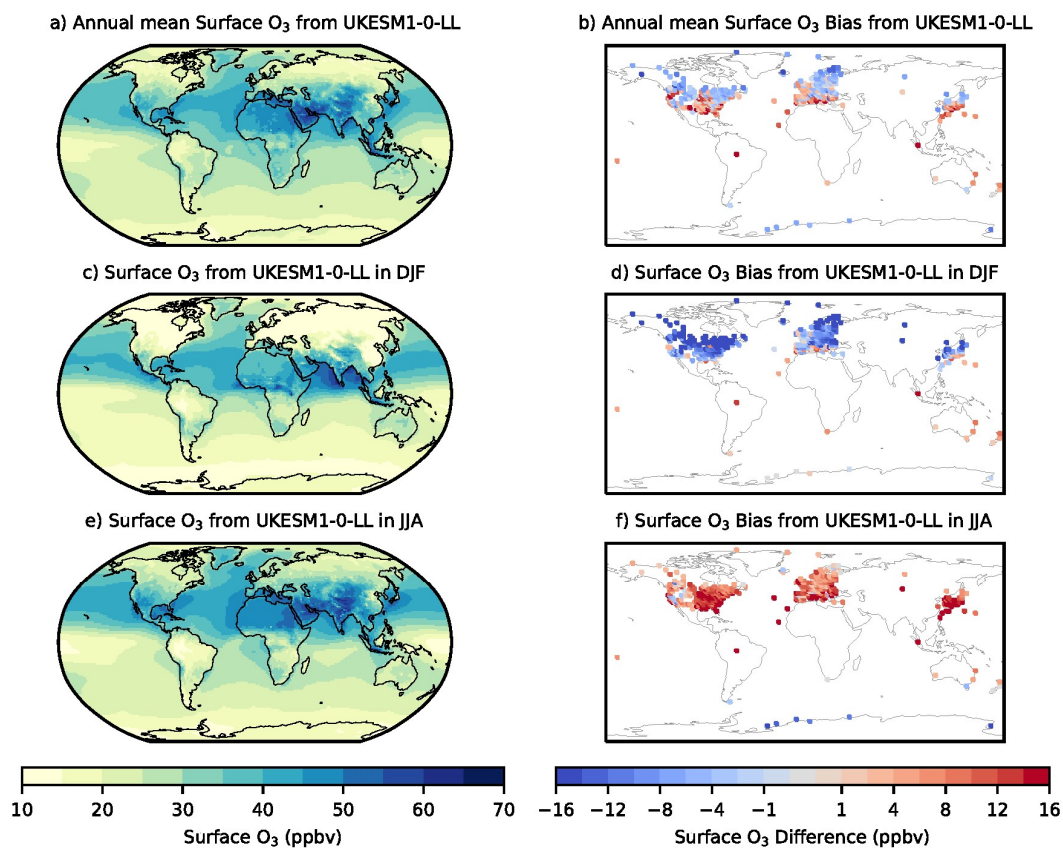
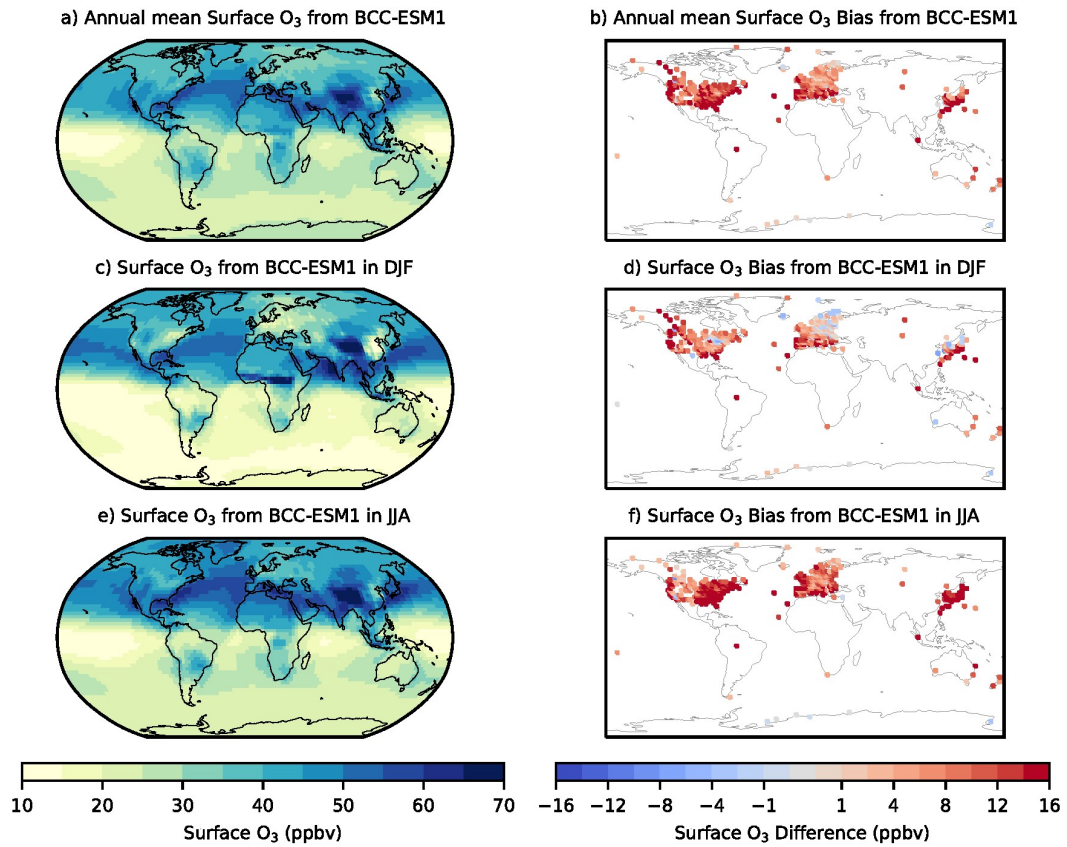


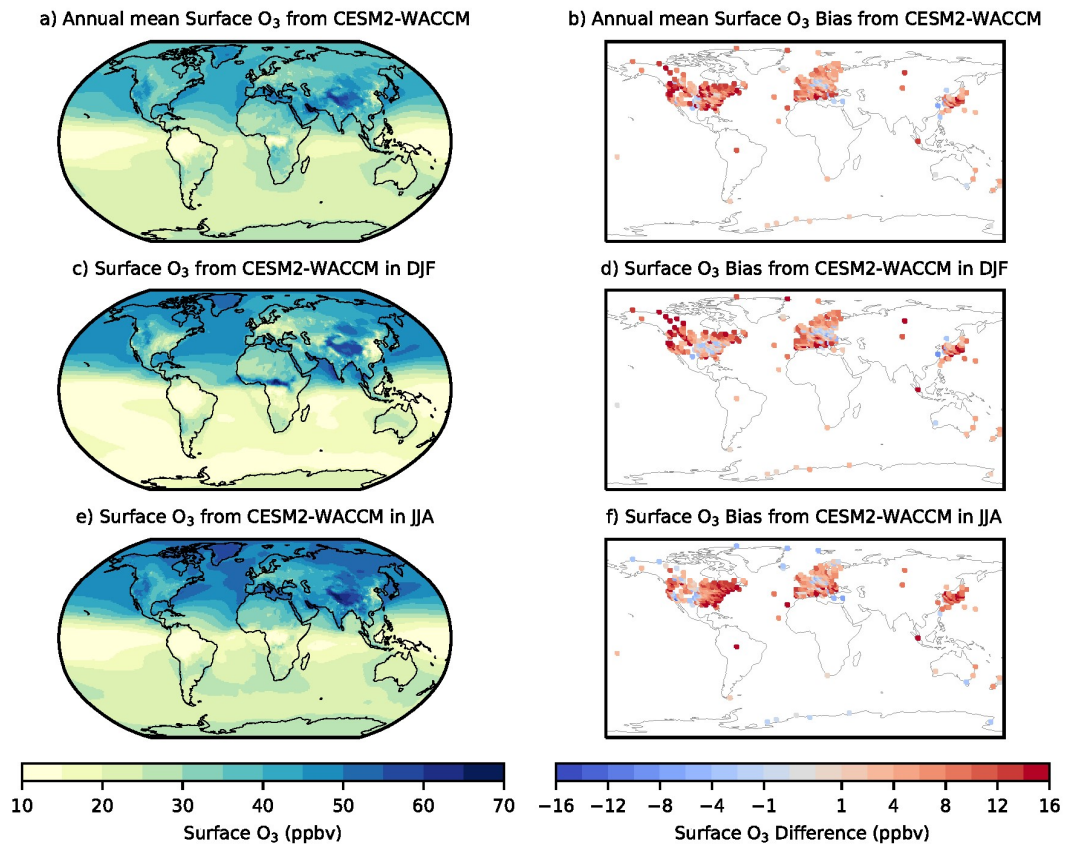
Figure S1 – Definition of regions used in the study, based on those used in Phase 2 of the Hemispheric Transport of Air Pollutants (HTAP2)



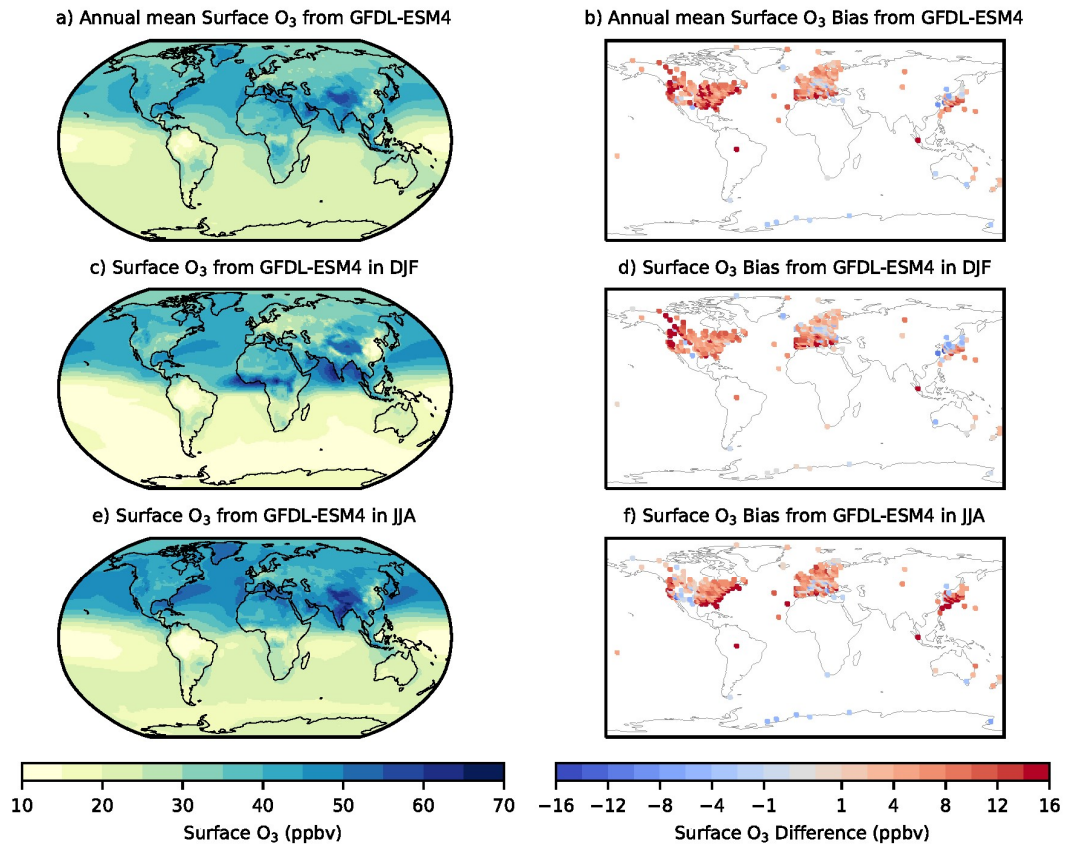
50 Figure S2 – Annual and seasonal mean surface O₃ concentrations from UKESM1-0-LL in a) Annual mean, c) December January, February (DJF) and e) June, July, August (JJA) over the 2005-2014 period. Difference between the UKESM1 mean and TOAR observations for b) Annual mean, d) DJF and f) JJA.



55 **Figure S3 – Annual and seasonal mean surface O₃ concentrations from BCC-ESM1 in a) annual mean, c) December January, February (DJF) and e) June, July, August (JJA) over the 2005-2014 period. Difference between the BCC-ESM1 mean and TOAR observations for b) annual mean, d) DJF and f) JJA.**



60 **Figure S4 – Annual and seasonal mean surface O₃ concentrations from CESM2-WACCM in a) annual mean, c) December January, February (DJF) and e) June, July, August (JJA) over the 2005-2014 period. Difference between the CESM2-WACCM mean and TOAR observations for b) Annual mean, d) DJF and f) JJA.**



65 **Figure S5** – Annual and seasonal mean surface O₃ concentrations from GFDL-ESM4 in a) Annual mean, c) December January, February (DJF) and e) June, July, August (JJA) over the 2005-2014 period. Difference between the GFDL-ESM4 mean and TOAR observations for b) Annual mean, d) DJF and f) JJA.

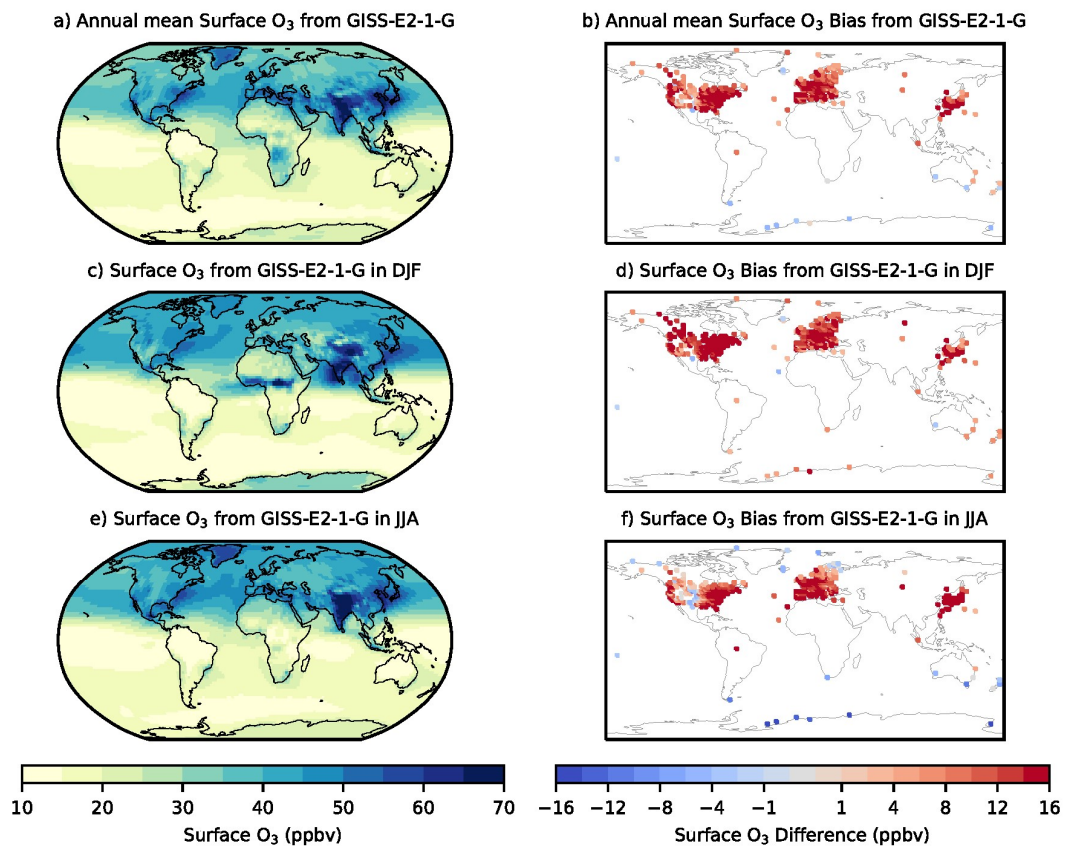
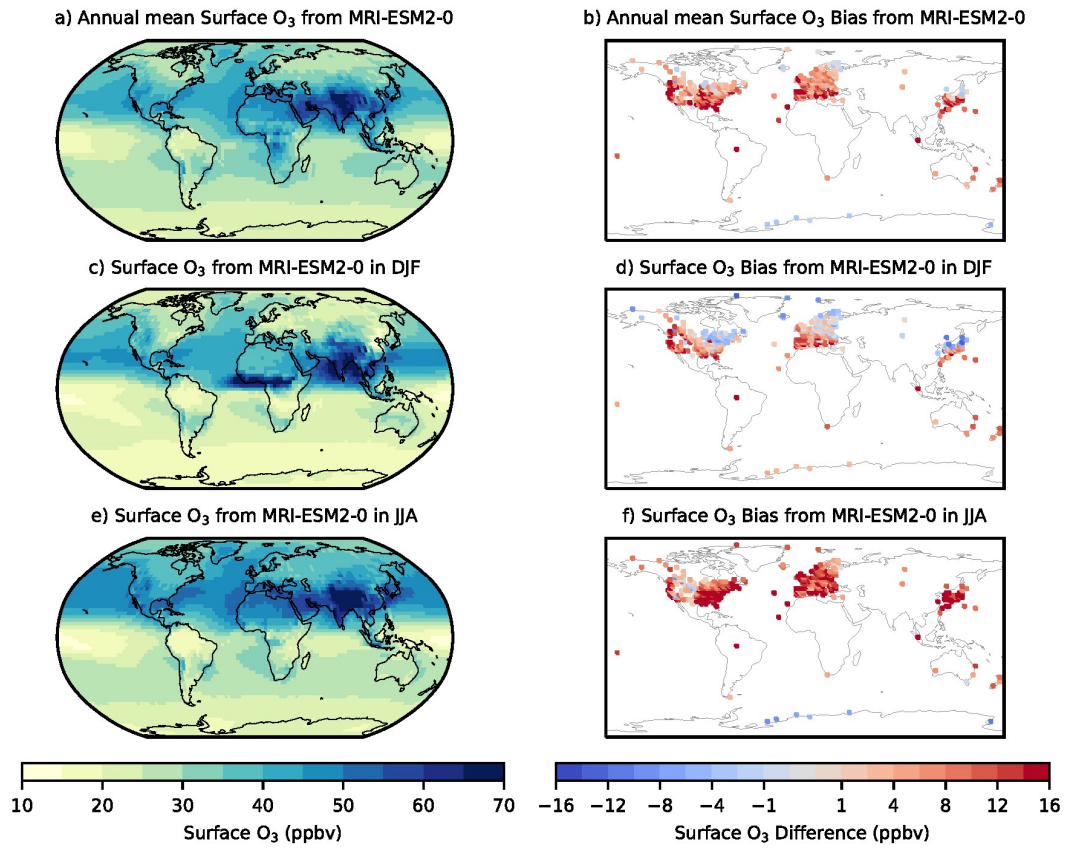
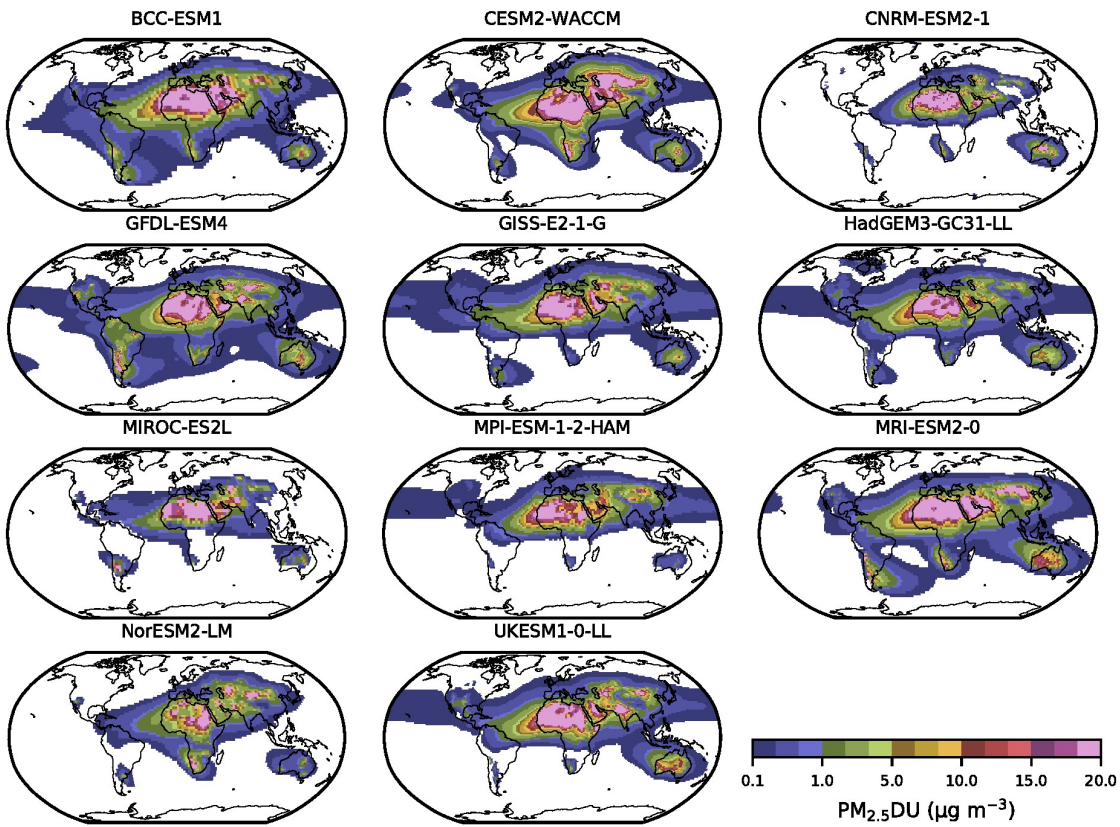


Figure S6 – Annual and seasonal mean surface O₃ concentrations from GISS-E2-1-G in a) Annual mean, c) December January, February (DJF) and e) June, July, August (JJA) over the 2005-2014 period. Difference between the GISS-E2-1-G mean and TOAR observations for b) Annual mean, d) DJF and f) JJA.



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Figure S7 – Annual and seasonal mean surface O₃ concentrations from MRI-ESM2-0 in a) Annual mean, c) December January, February (DJF) and e) June, July, August (JJA) over the 2005-2014 period. Difference between the MRI-ESM2-0 mean and TOAR observations for b) Annual mean, d) DJF and f) JJA.



75 Figure S8 – Annual mean PM_{2.5} dust component calculated for each individual CMIP6 model over the period 2005-2014

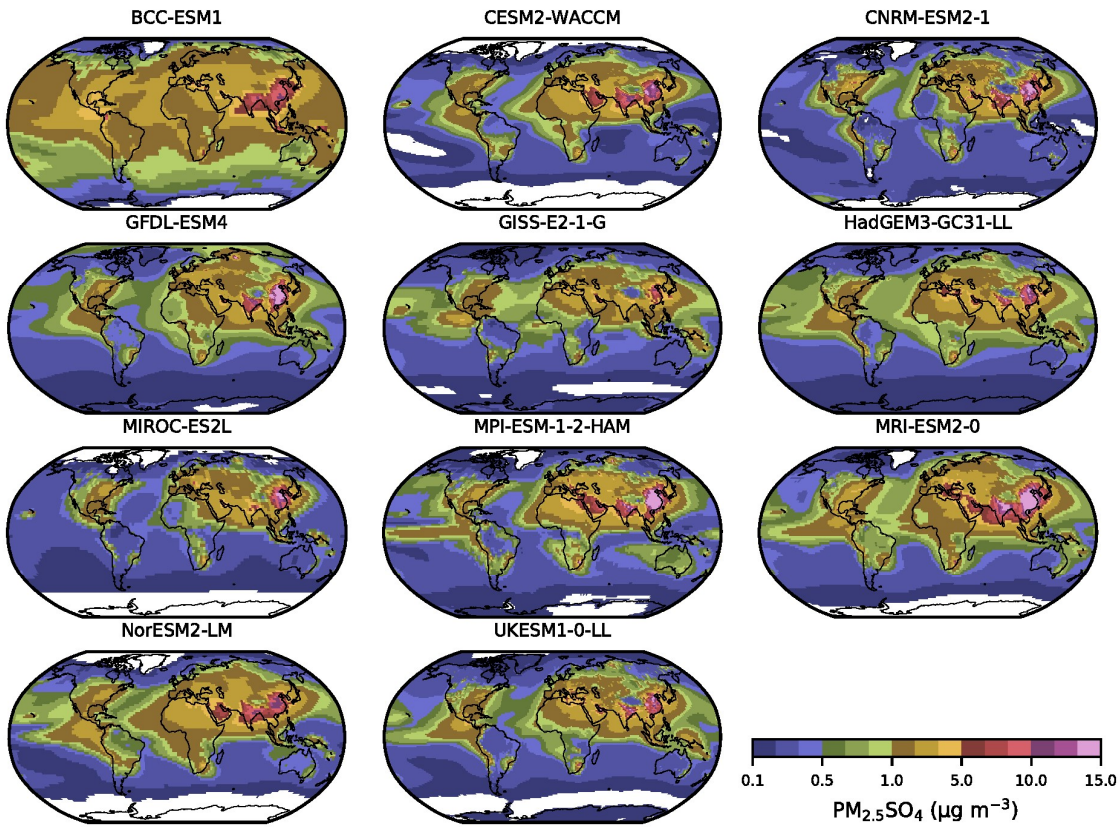


Figure S9 – Annual mean $PM_{2.5} SO_4$ component calculated for each individual CMIP6 model over the period 2005-2014

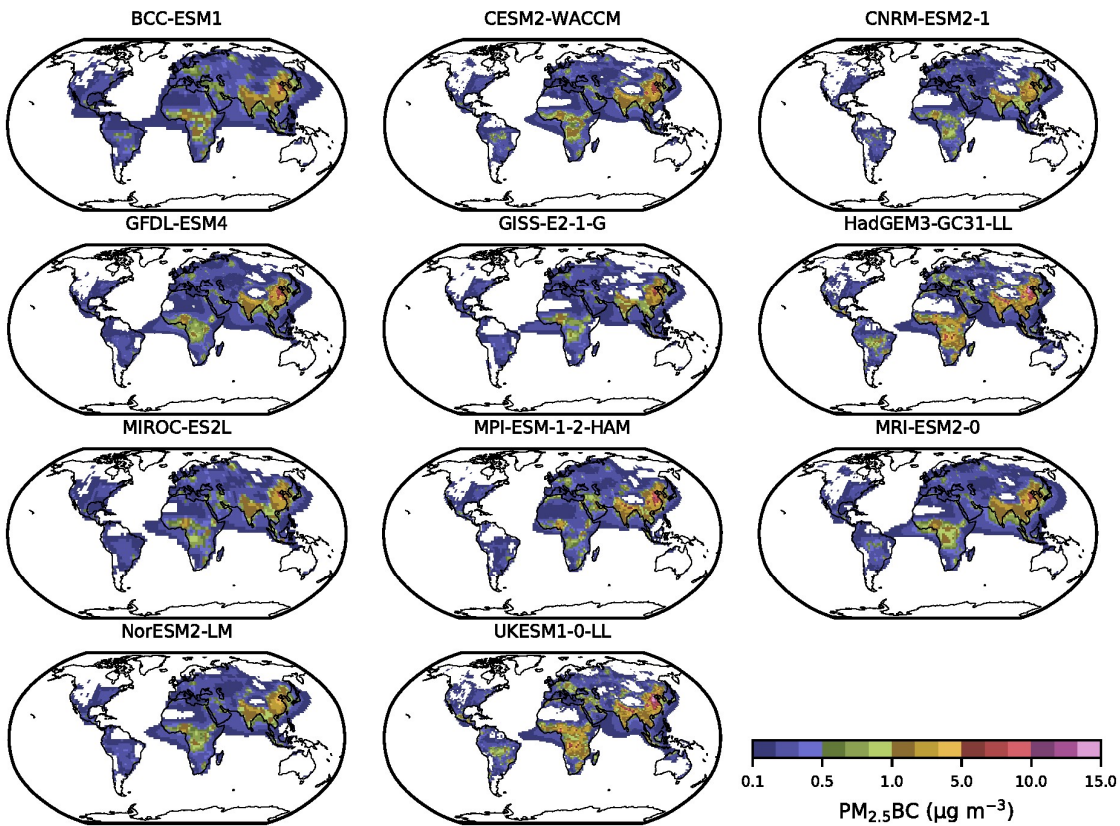
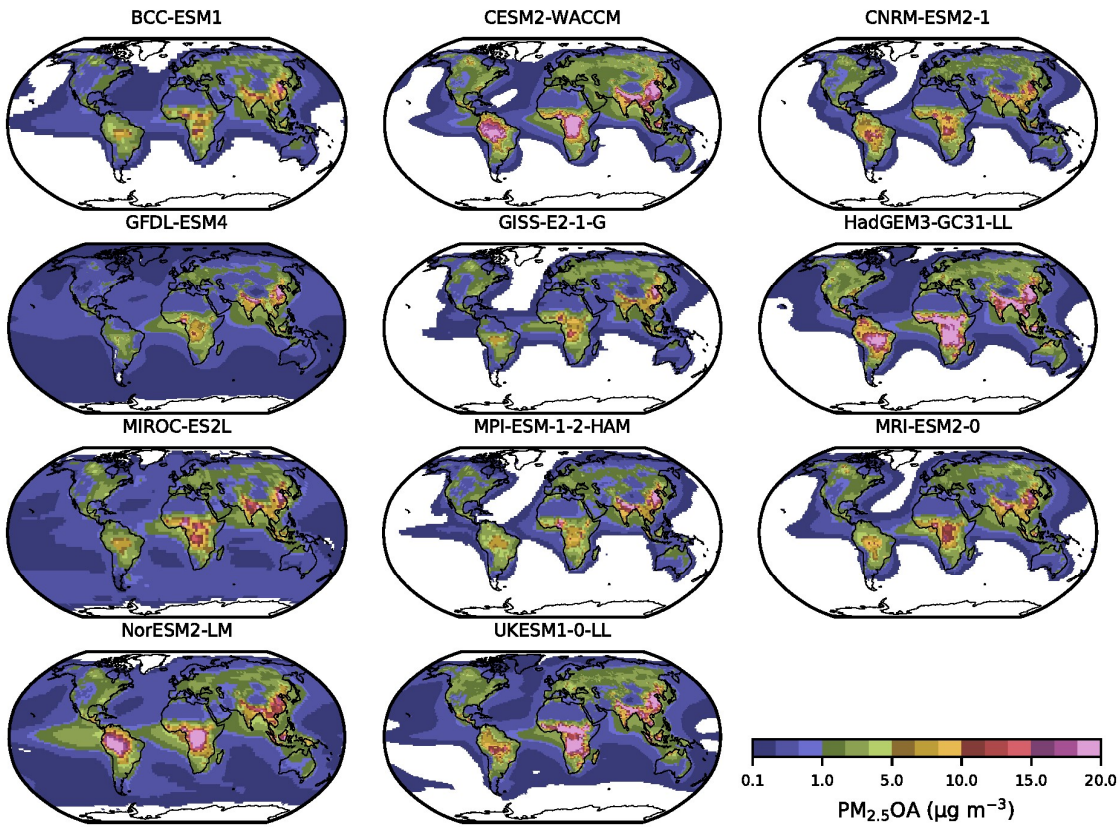


Figure S10 – Annual mean $PM_{2.5} BC$ component calculated for each individual CMIP6 model over the period 2005-2014



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Figure S11 – Annual mean $PM_{2.5}$ OA component calculated for each individual CMIP6 model over the period 2005-2014

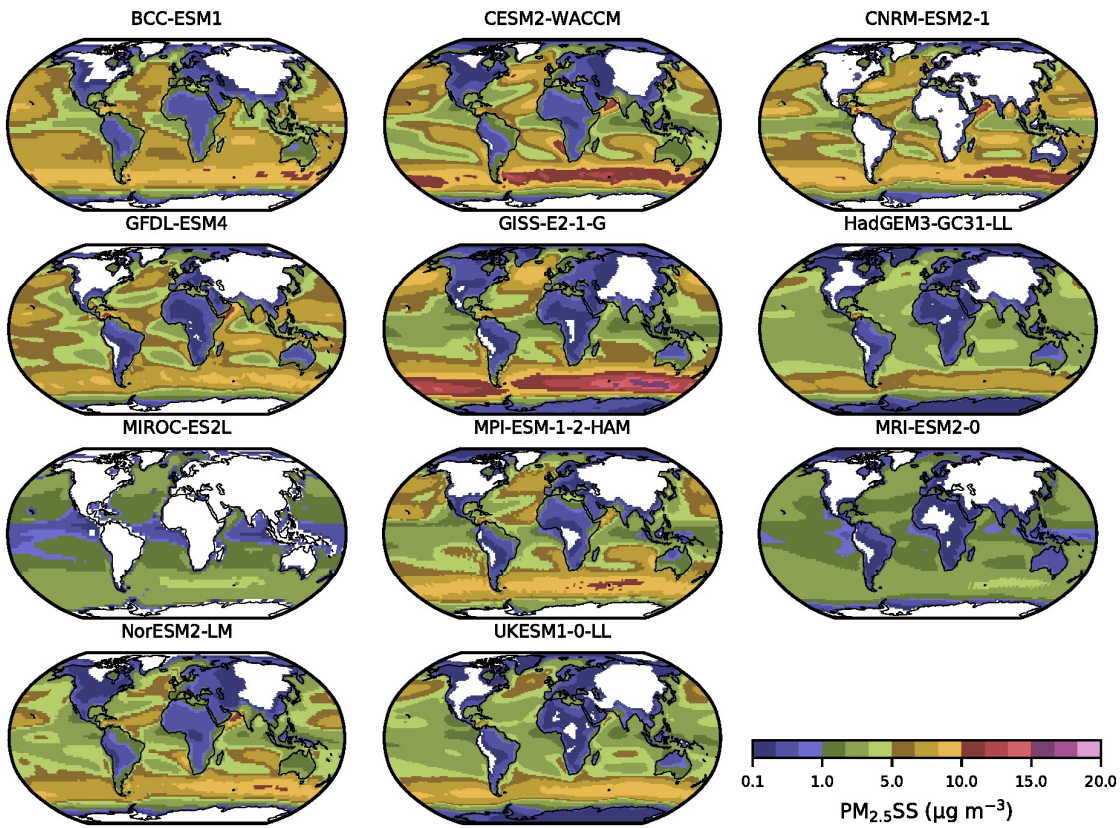
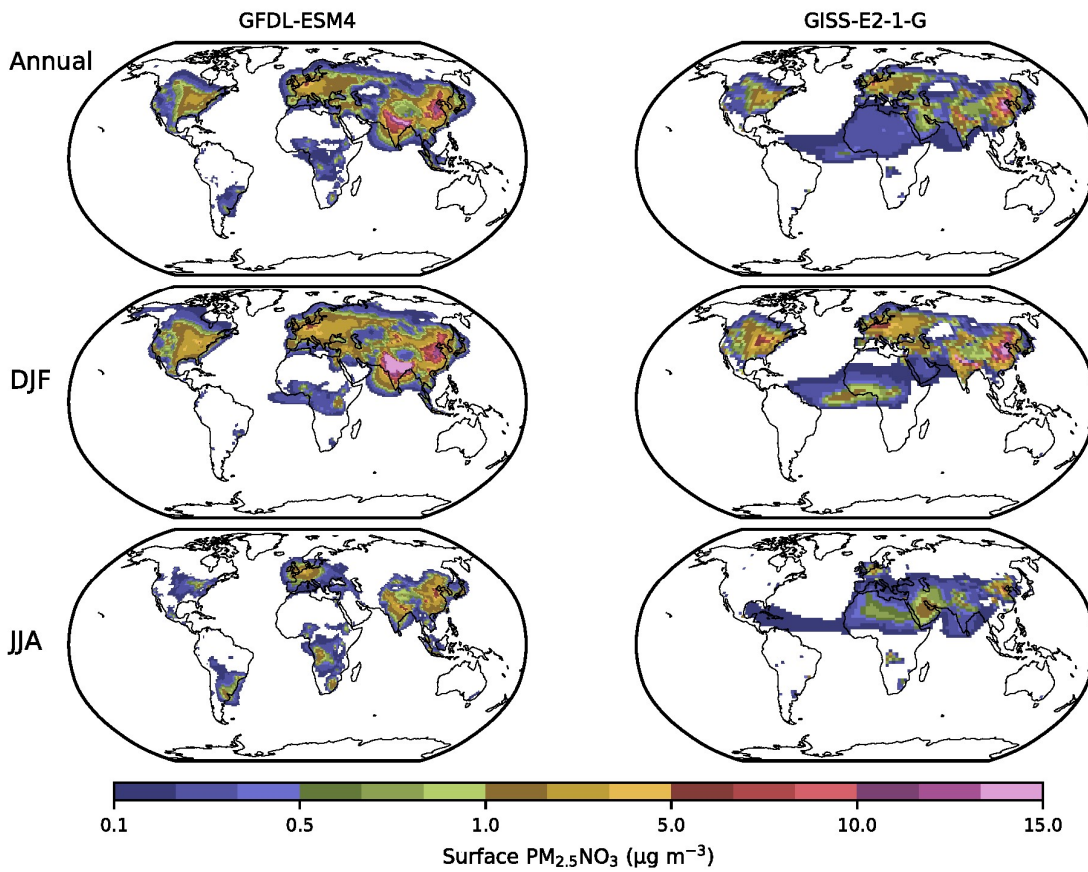
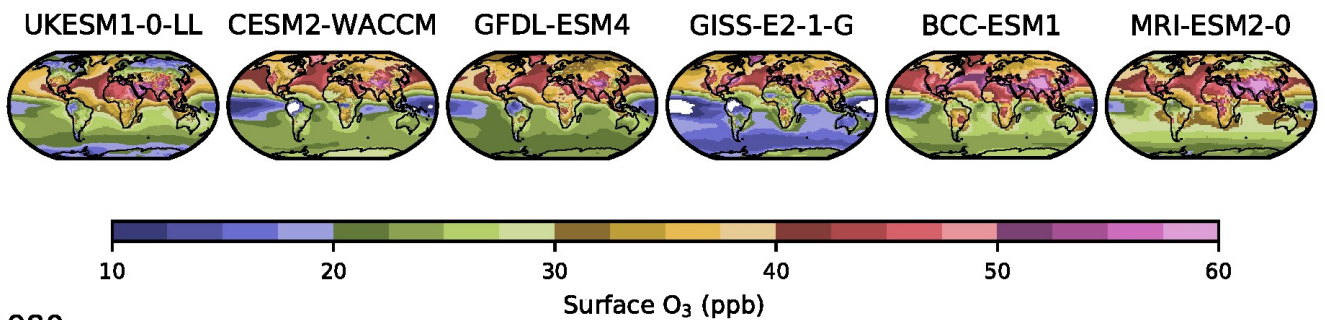


Figure S12 – Annual mean $PM_{2.5}$ SS (sea salt) component calculated for each individual CMIP6 model over the period 2005-2014



85 Figure S13 – Annual and seasonal mean $PM_{2.5}NO_3$ (nitrate) component calculated for each individual CMIP6 model that made the data available over the period 2005-2014

2005-14



1980



1850

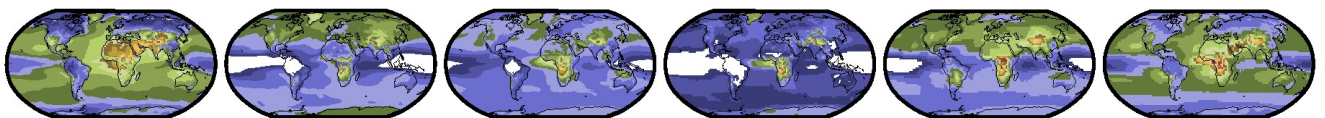
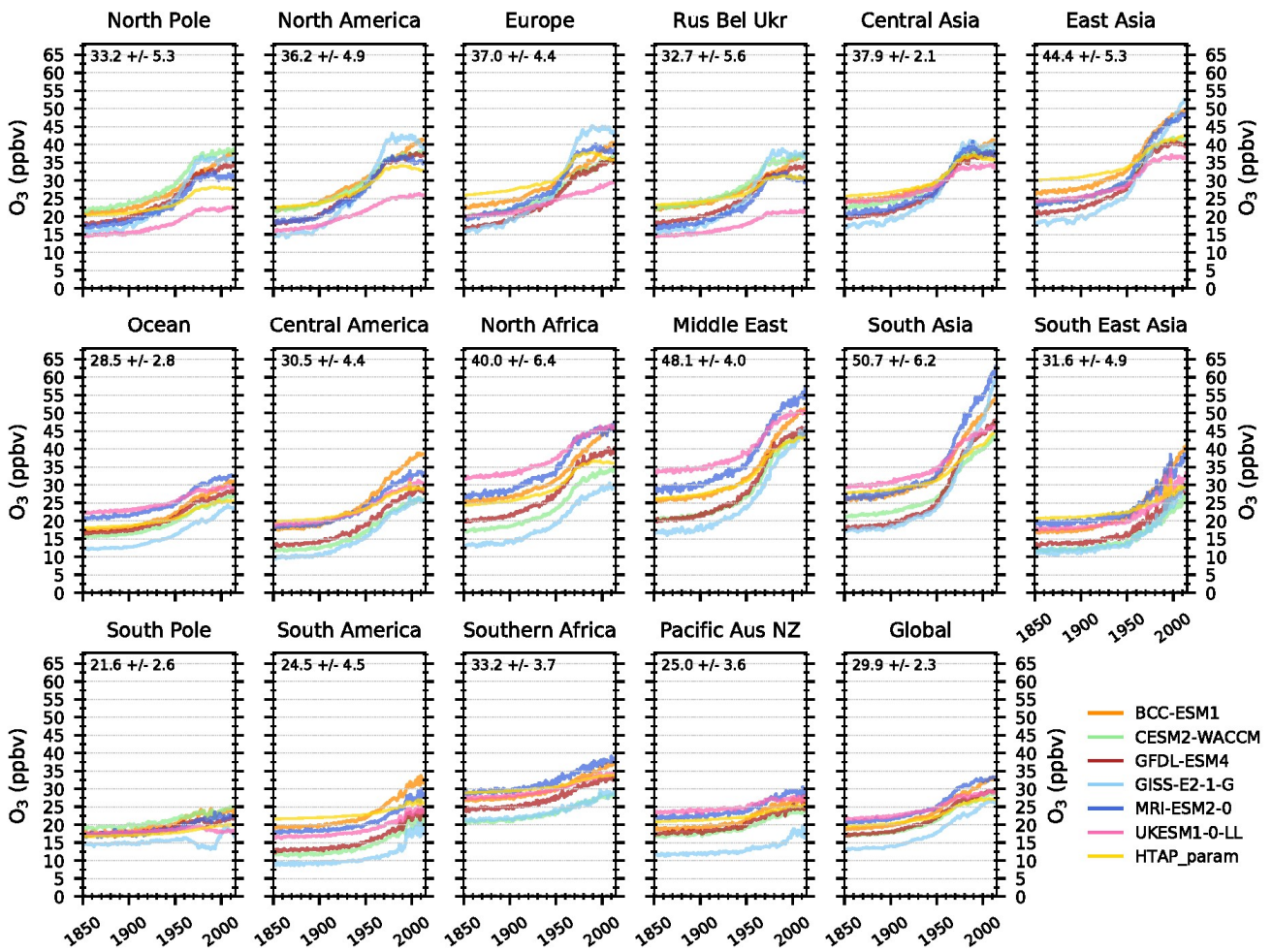
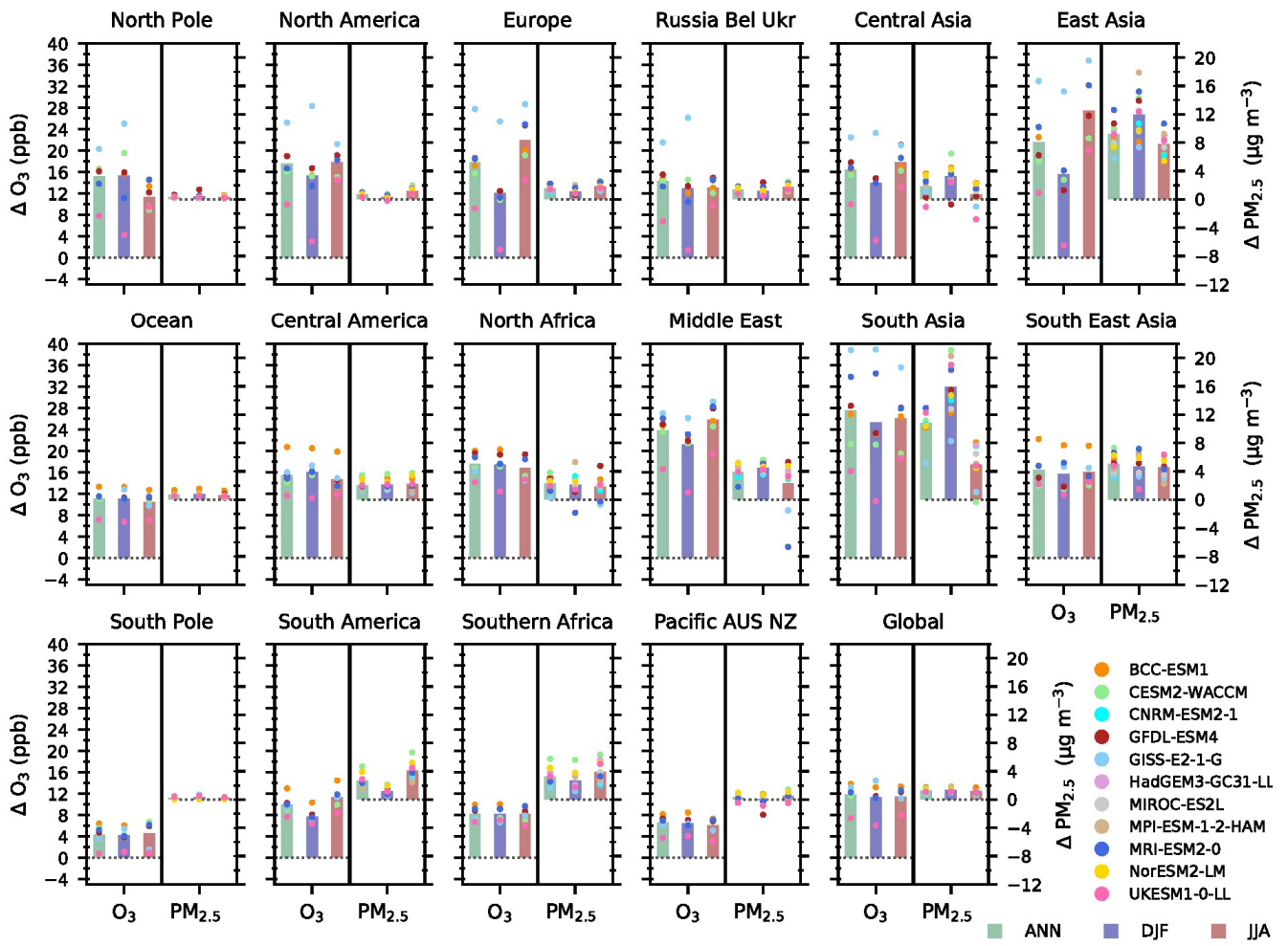


Figure S14 - Annual mean surface O_3 concentrations across 6 CMIP6 models over the period 2005-2014 (top row), 1980-1989 (middle row) and 1850-1859 (bottom row).

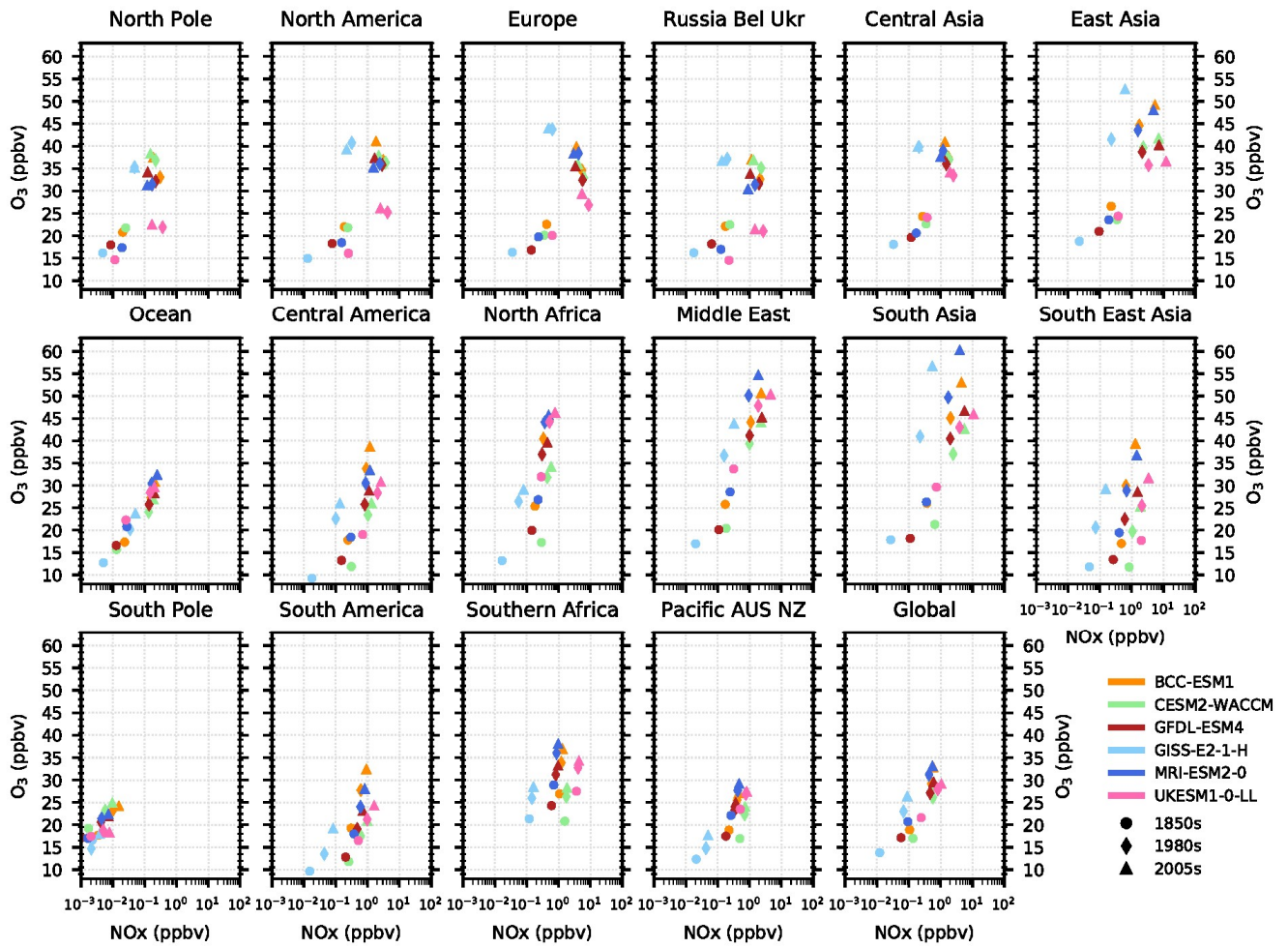


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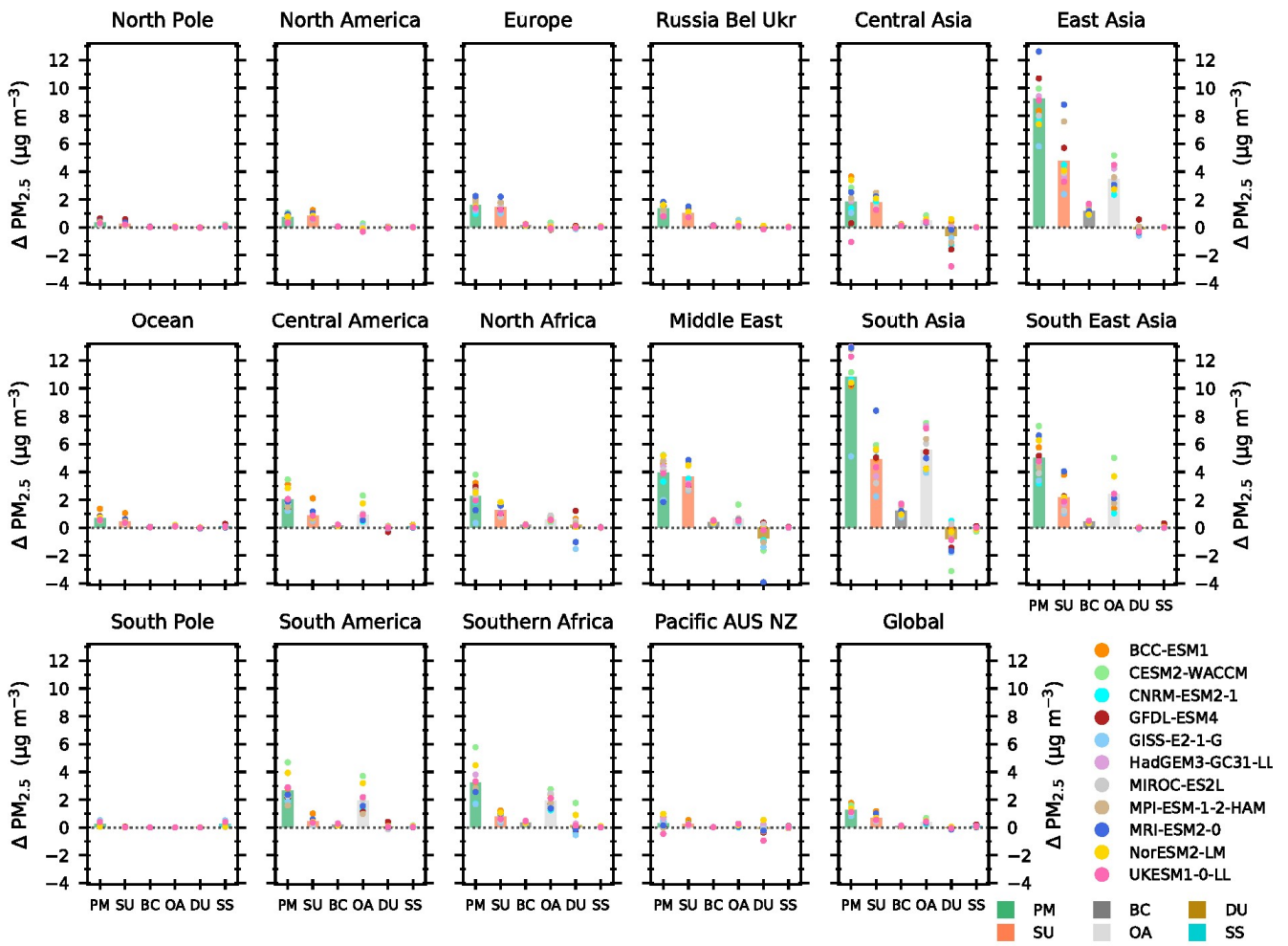
Figure S15 - Regional and global annual mean surface O₃ concentrations across 6 CMIP6 models and the HTAP_param. The multi-model annual mean year 2005-2014 surface O₃ concentrations (+/- 1 standard deviation) are shown in the top left of each panel. Regions are defined in Figure S1.



95 Figure S16 – Annual and seasonal regional mean changes in surface O_3 and $PM_{2.5}$ from pre-industrial (1850-1859 mean) to present day (2005-2014 mean) across 11 CMIP6 models for $PM_{2.5}$ and 6 models for O_3 . Individual circles represent each annual and seasonal mean change from individual CMIP6 models, with the multi-model mean represented by the solid bar.

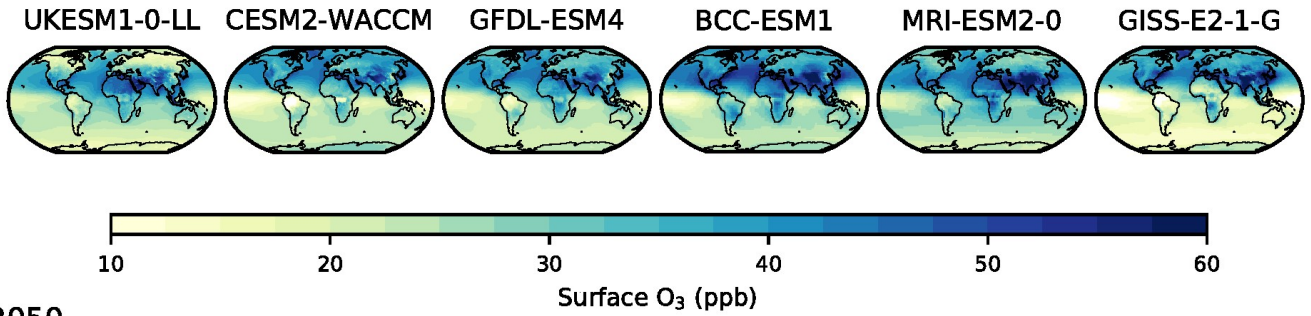


100 Figure S17 – Annual mean regional surface O_3 concentrations compared to regional annual mean surface NO_x ($NO + NO_2$) concentrations across 6 CMIP6 models over three ten-year periods of 1850-1859 (circles), 1980-1989 (diamonds) and 2005-2014 (triangle).

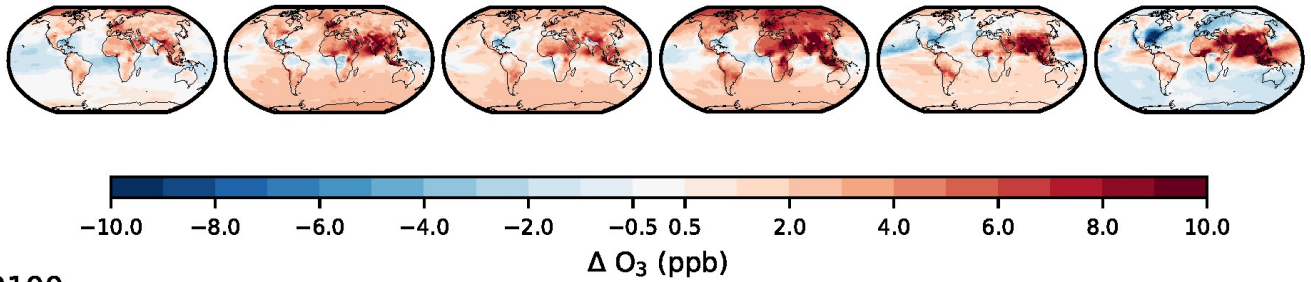


105 Figure S18 – Pre-industrial (1850-1859 mean) to present day (2005-2014 mean) changes in the regional and global annual mean surface $PM_{2.5}$ concentrations (PM) and that from each individual component (BC – black carbon, DU – dust, SU – sulphate, OA – organic aerosol and SS – sea salt). Individual circles represent each annual and seasonal mean changes from the 11 individual CMIP6 models, with the multi-model mean represented by the solid bar. The Regions are defined in Figure S1.

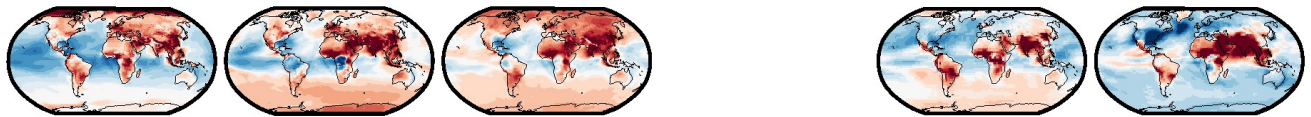
2005-14



2050

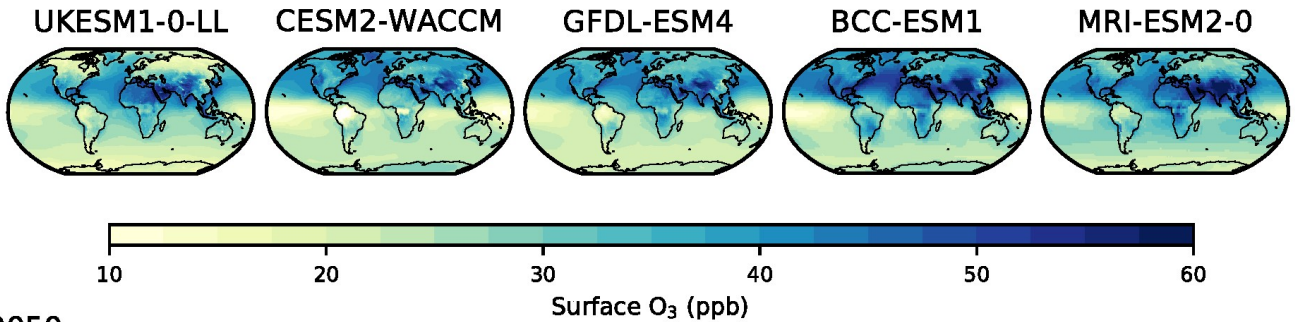


2100

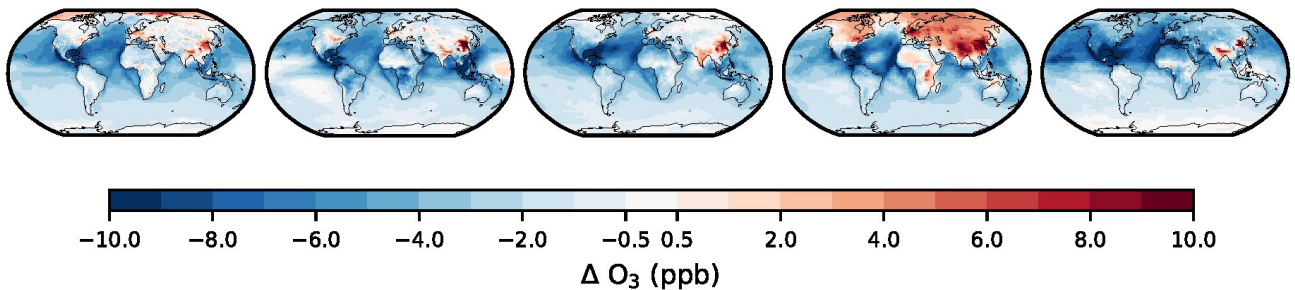


110 Figure S19 – Annual mean surface O₃ concentrations and future response in ssp370 across 6 different CMIP6 models. Top row shows the 2005-2014 annual mean surface O₃ concentrations in each model from the historical simulations. Middle row shows the surface O₃ response in 2050, relative to 2005-2014 mean, in each model for ssp370. Bottom row shows the same as the middle but for 2100. No data is presented in 2100 for BCC-ESM1 as data for ssp370 only extended out to 2055.

2005-14

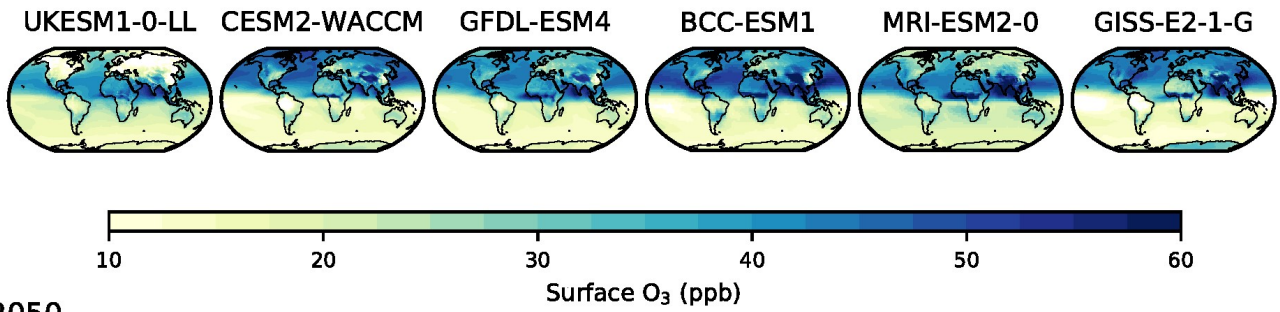


2050

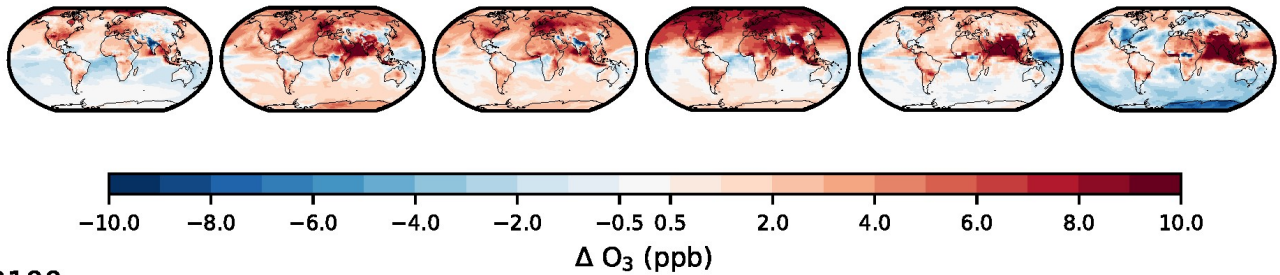


115 Figure S20 - Annual mean surface O₃ concentrations and future response in ssp370-lowNTCF across five different CMIP6 models. Top row shows the 2005-2014 annual mean surface O₃ concentrations in each model from the historical simulations. Bottom row shows the surface O₃ response in 2050, relative to the 2005-2014 mean, in each model for ssp370-lowNTCF.

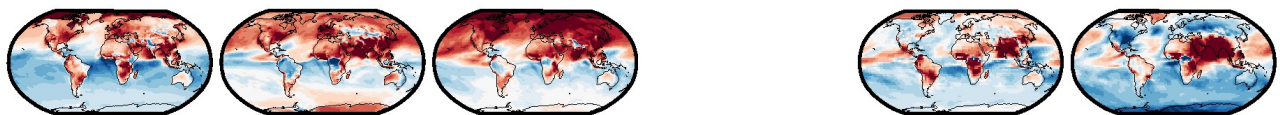
2005-14



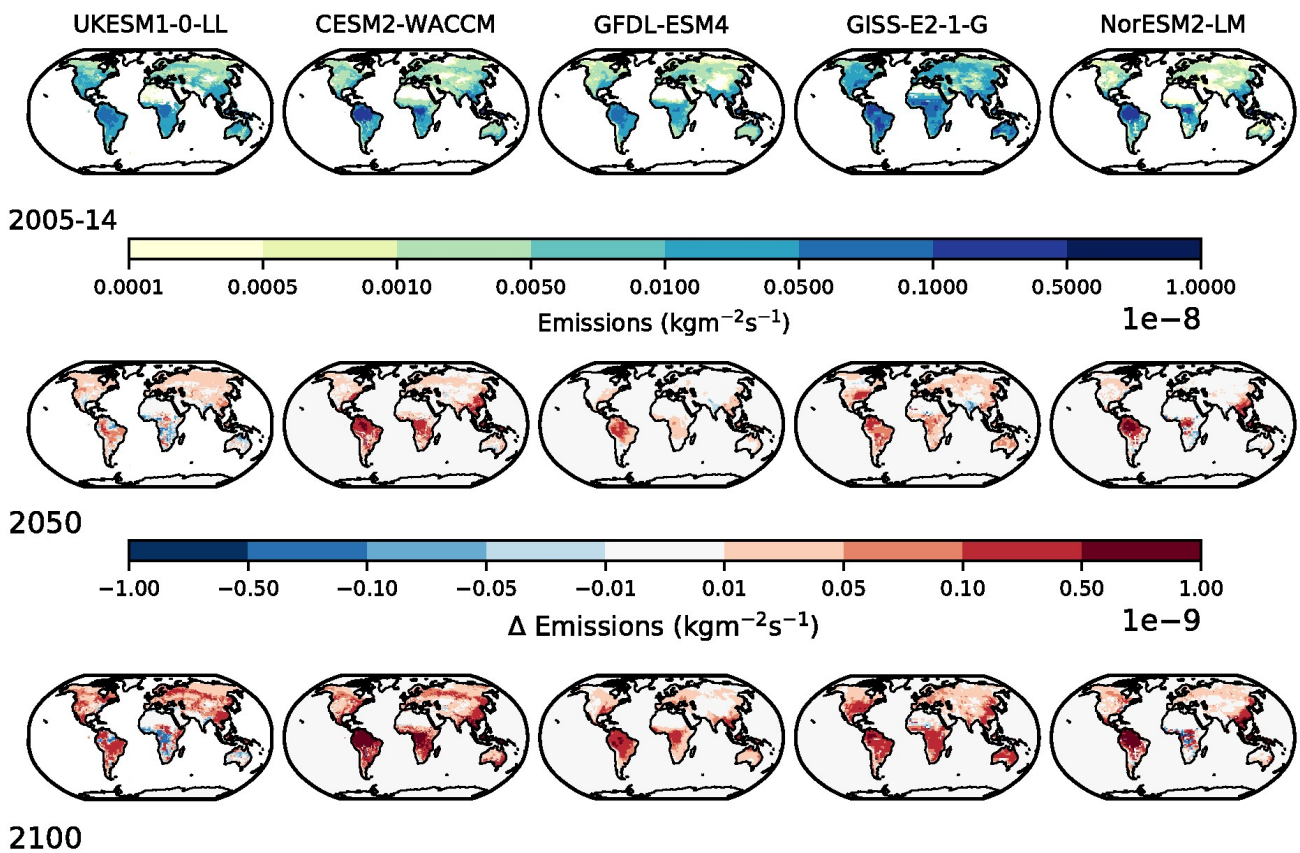
2050



2100



120 Figure S21 – December January February (DJF) mean surface O₃ concentrations and future response in ssp370 across 6 different CMIP6 models. Top row shows the 2005-2014 DJF mean surface O₃ concentrations in each model from the historical simulations. Middle row shows the surface DJF O₃ response in 2050, relative to 2005-2014 mean, in each model for ssp370. Bottom row shows the same as the middle but for 2100. No data is presented in 2100 for BCC-ESM1 as data for ssp370 only extended out to 2055.



125 Figure S22 – Annual mean emissions of total biogenic volatile organic compounds across 5 CMIP6 models. Top row shows the 2005-2014 annual mean emissions in each model from the historical simulations. Middle row shows the change in emissions in 2050, relative to 2005-2014 mean, in each model for ssp370. Bottom row shows the same as the middle but for 2100. The total BVOC emissions from each model includes a different number of individual BVOC species (Table S1).

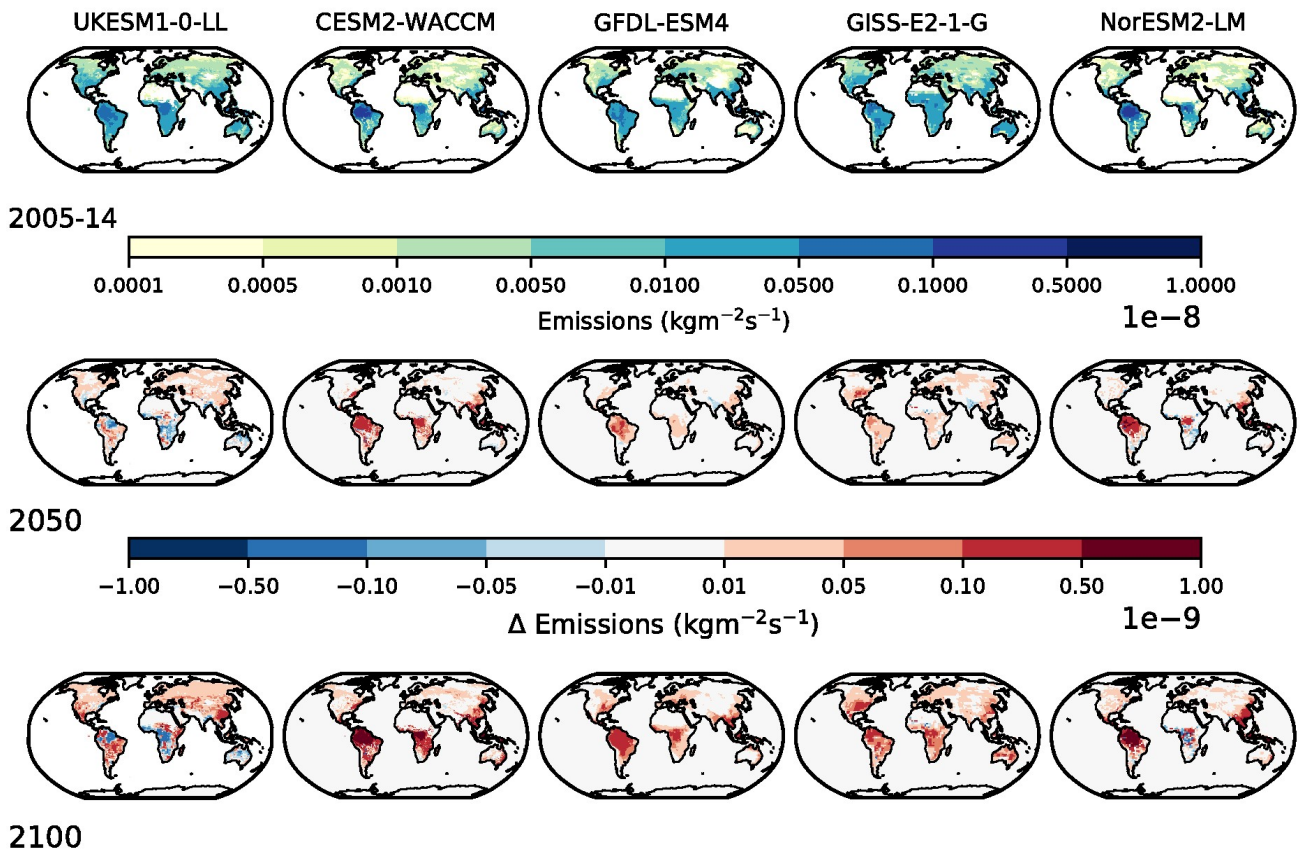


Figure S23 – Annual mean emissions of isoprene across 5 CMIP6 models. Top row shows the 2005-2014 annual mean emissions in each model from the historical simulations. Middle row shows the change in emissions in 2050, relative to 2005-2014 mean, in each model for ssp370. Bottom row shows the same as the middle but for 2100.

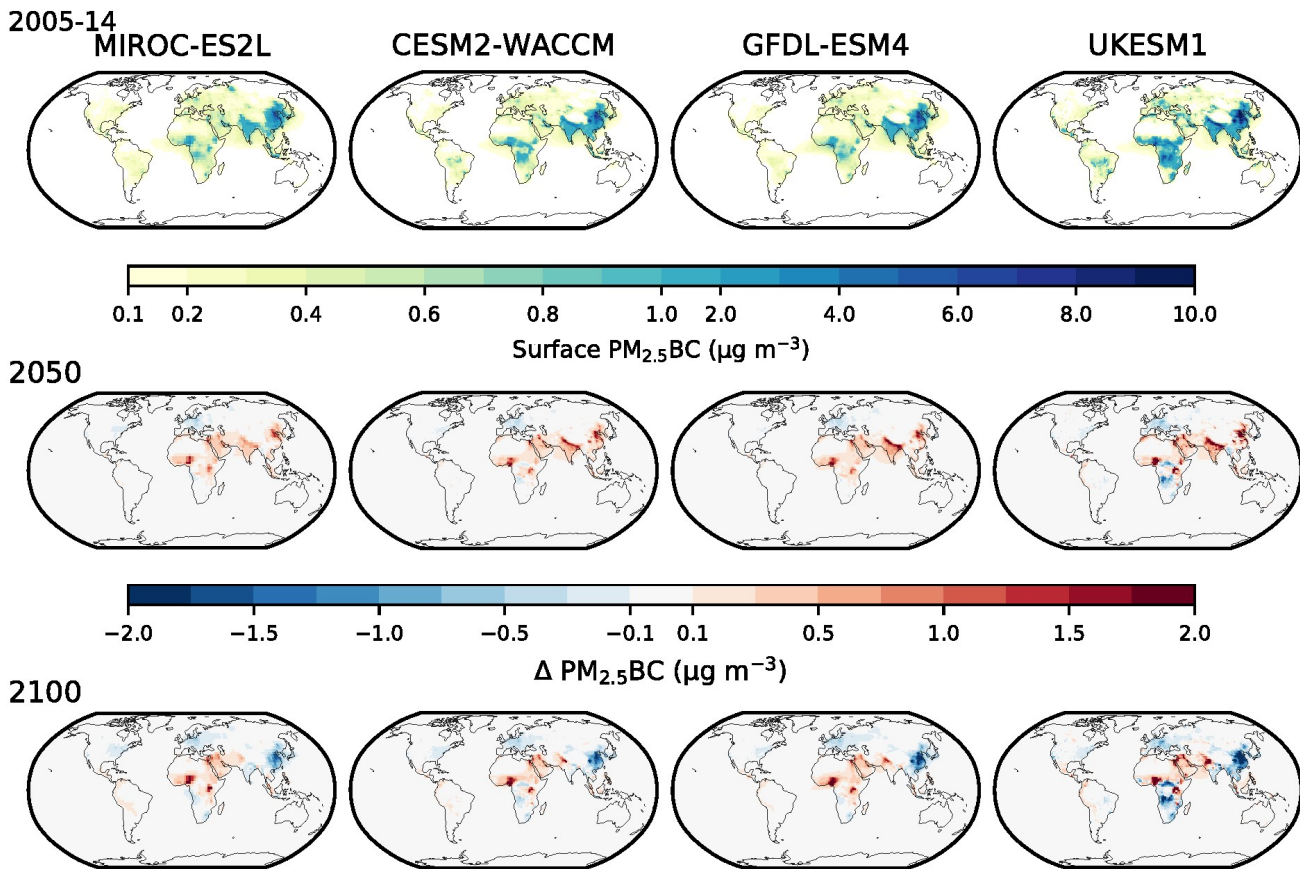
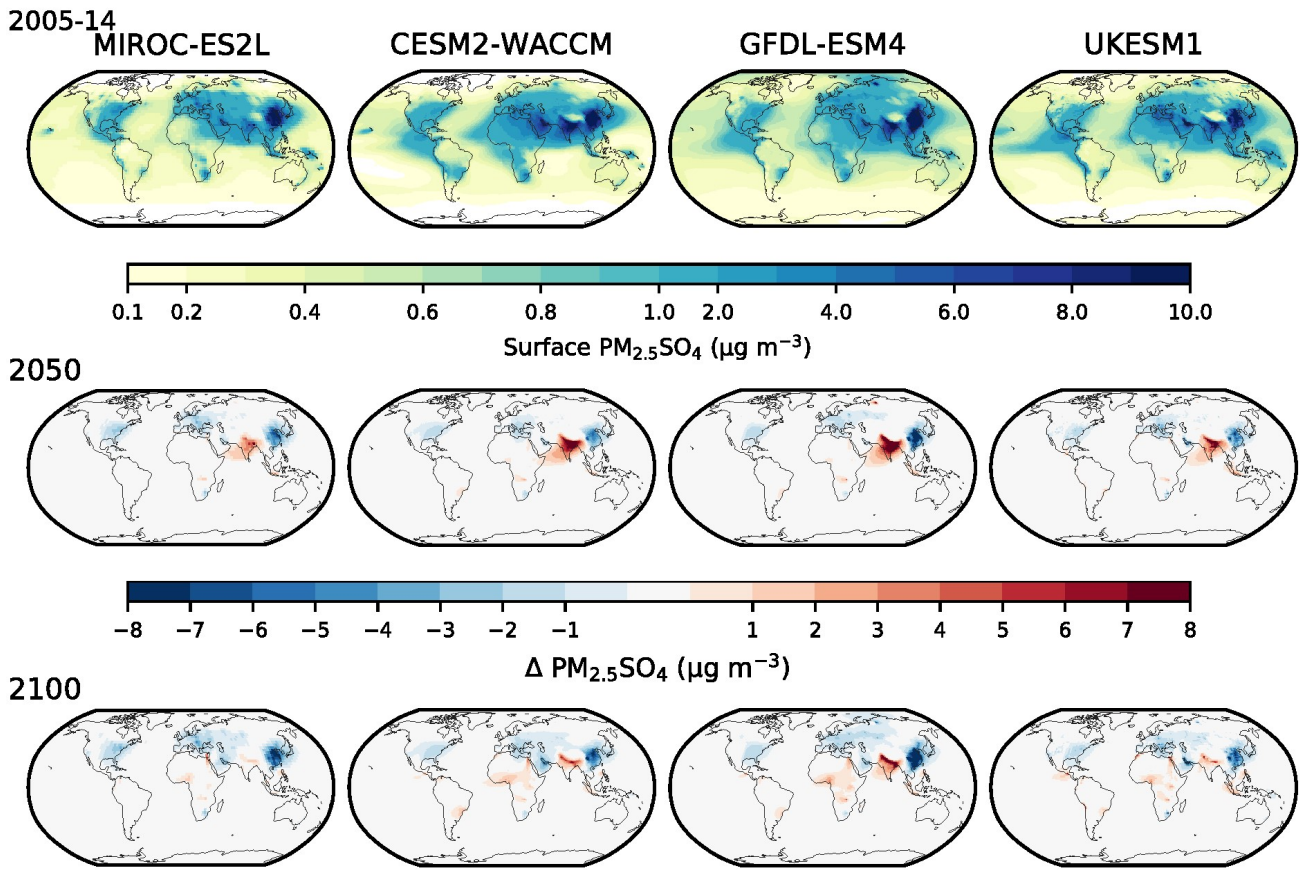


Figure S24 – Annual mean surface PM_{2.5} black carbon concentrations and future response in ssp370 across four different CMIP6 models. Top row shows the 2005-2014 annual mean surface PM_{2.5} black carbon concentrations in each model from the historical simulations. Middle row shows the decadal mean surface PM_{2.5} black carbon response in 2050 (2045-2055), relative to 2005-2014 mean, in each model for ssp370. Bottom row shows the same as the middle but for 2095 (2090-2100).



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Figure S25 – same as Fig S24 but for $PM_{2.5}$ sulphate

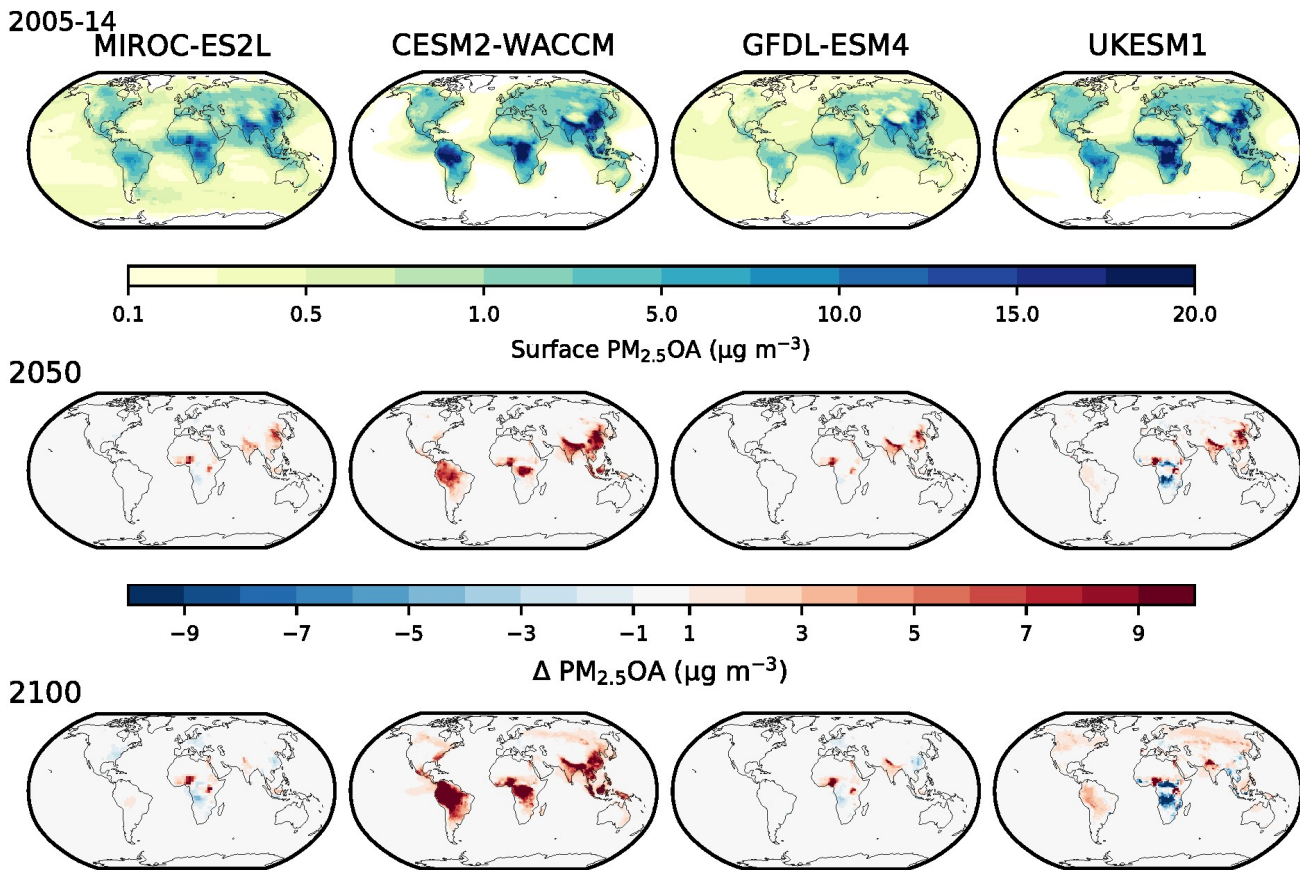
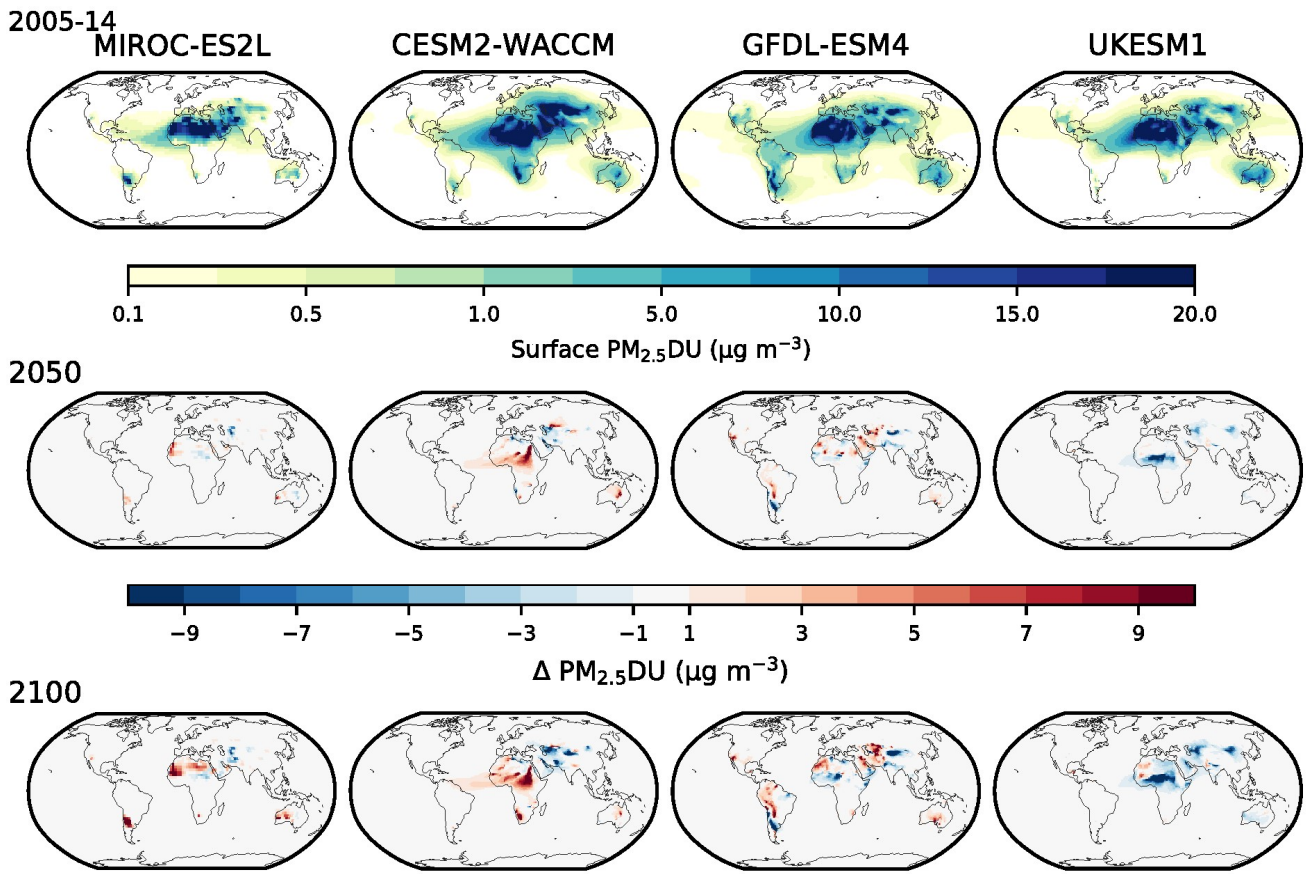


Figure S26 – same as Fig S24 but for $PM_{2.5}$ organic aerosol



140 Figure S27 – same as Fig S24 but for $PM_{2.5}$ dust

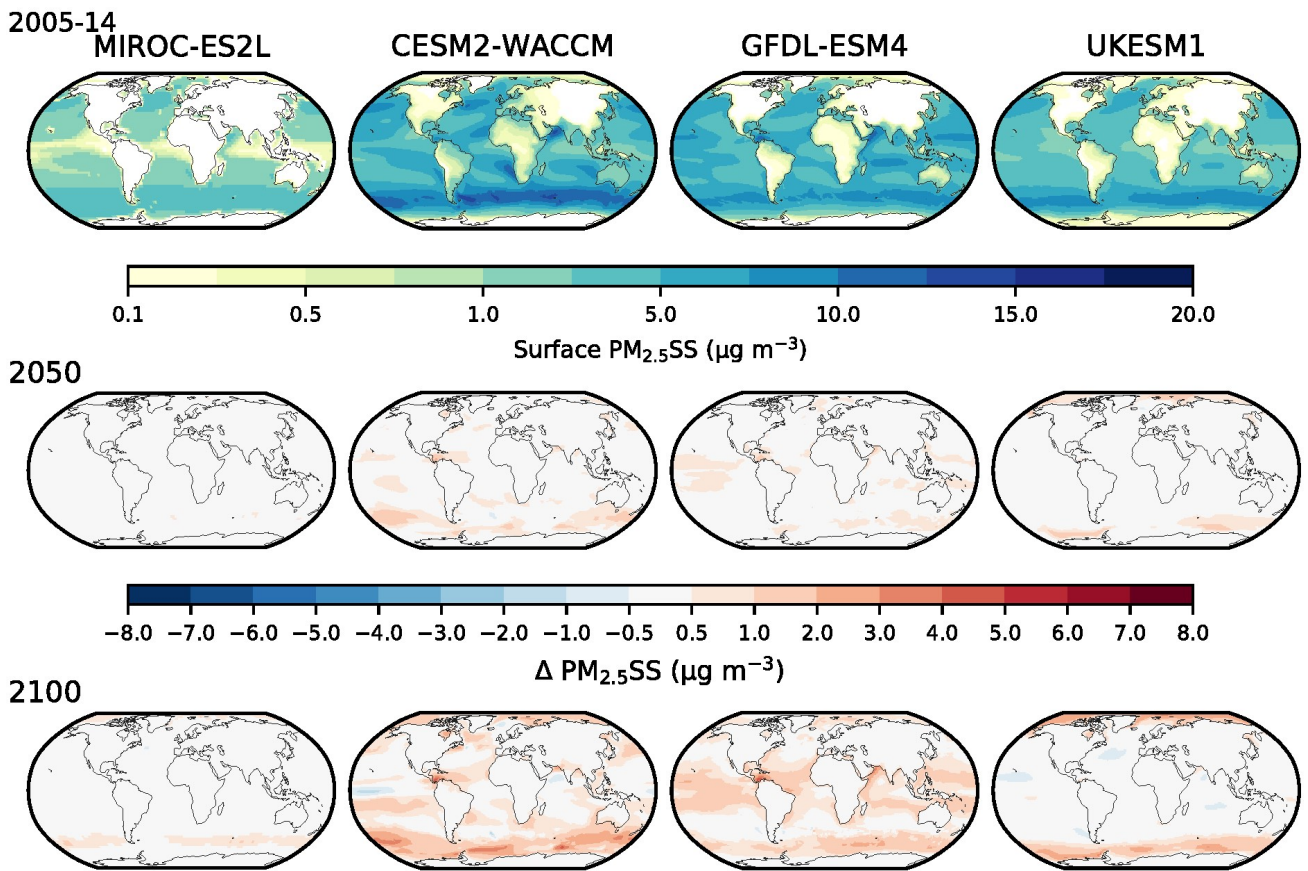


Figure S28 – same as Fig S24 but for $PM_{2.5}$ sea salt