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Large simulated future changes in the nitrate radical under the CMIP6 SSP scenarios: implications for oxidation chemistry

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S1. Corrections to the NO_3+Monoterp reaction in UKESM1

As described in the Methods section of the main paper, the reaction rate coefficient for the NO_3+Monoterp reaction was corrected. Here we present the changes to the global chemistry from this change in reaction rate coefficient. In the figures below, the "Old" simulations use the incorrect reaction rate constant of $k_{NO_3} = 1.19 \times 10^{-12} \times e^{(925/T)}$; whereas the "New" simulations use $k^*_{NO_3} = 1.19 \times 10^{-12} \times e^{(490/T)}$, resulting in a roughly four-fold decrease in reaction rate at 298 K. Figure S1 shows the change in concentrations of O_3, NO_2 and NO_3 in the lowest km of the atmosphere between simulations conducted with the Old and New reaction rate constants. Figure S2 and S3 shows changes in average flux through the NO_3+Monoterp reaction through the vertical column averaged over the globe and South Asia respectively. Correction to the NO_3+Monterp reaction rate constant results in an average reduction of the NO_3+Monoterp reaction flux of between 5 and 20% globally, depending on vertical level and scenario. Over the more polluted South Asia region, the reduction in flux can be over 30%. Changes to reaction flux are not as great as may be expected from the four-fold change in reaction rate coefficient because concentrations of Monoterp and NO_3 change in response, buffering the effect.

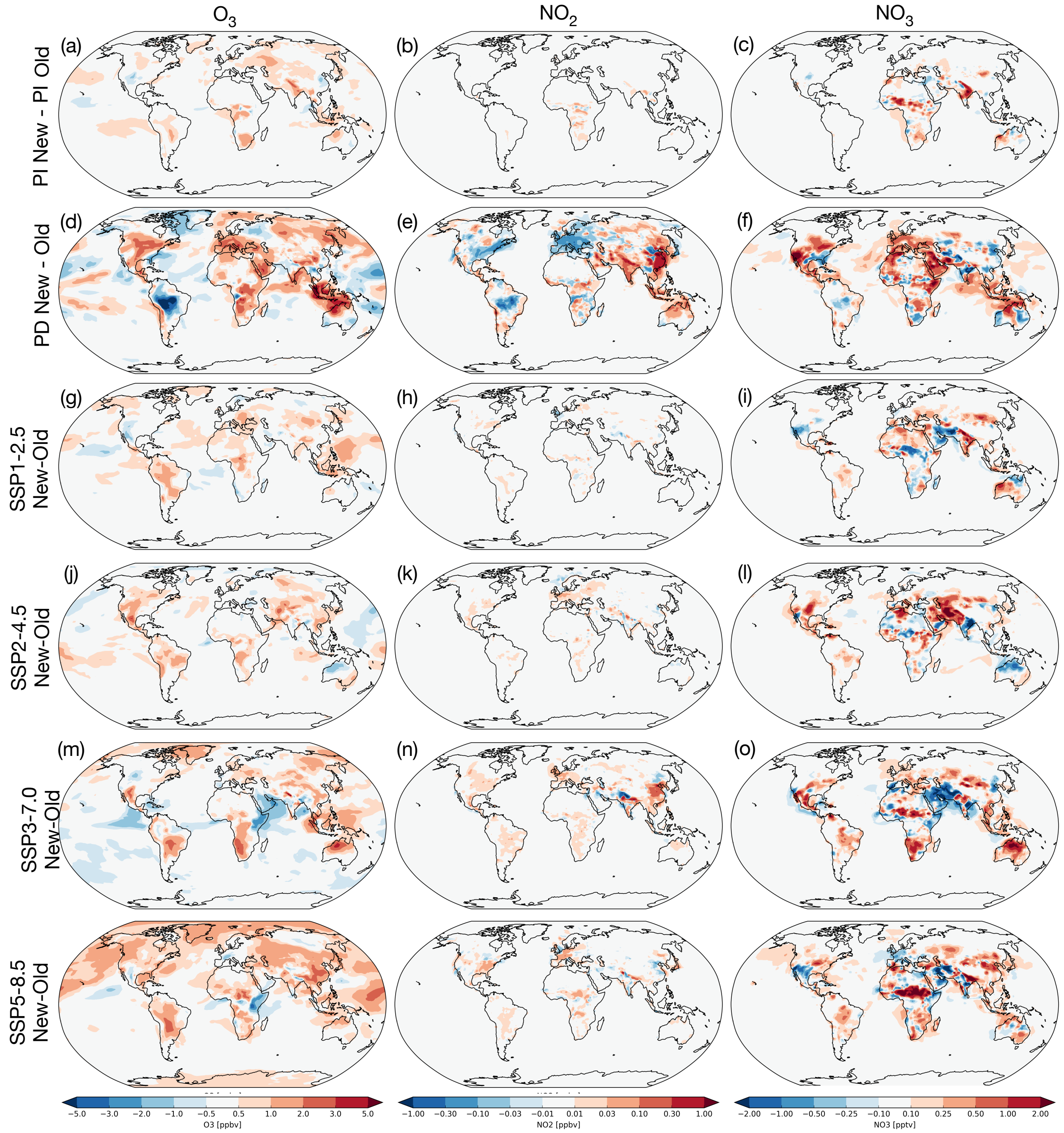

Fig. S1. Changes in O_3, NO_2 and NO_3 mixing ratios averaged over lowest 1km of the atmosphere. Showing difference between "new" simulations with updated NO_3+Monoterp reaction rate and "Old" using incorrect rate. Plots for Preindustrial (1850-1854) time period (a-c), Present Day (2010-2014) (d-f), SSP1-2.6 (2090-2094) (g-i), SSP2-4.5 (2090-2094) (j-l), SSP3-7.0 (2090-2094) (m-o) and SSP5-8.5 (2090-2094) (r-t).

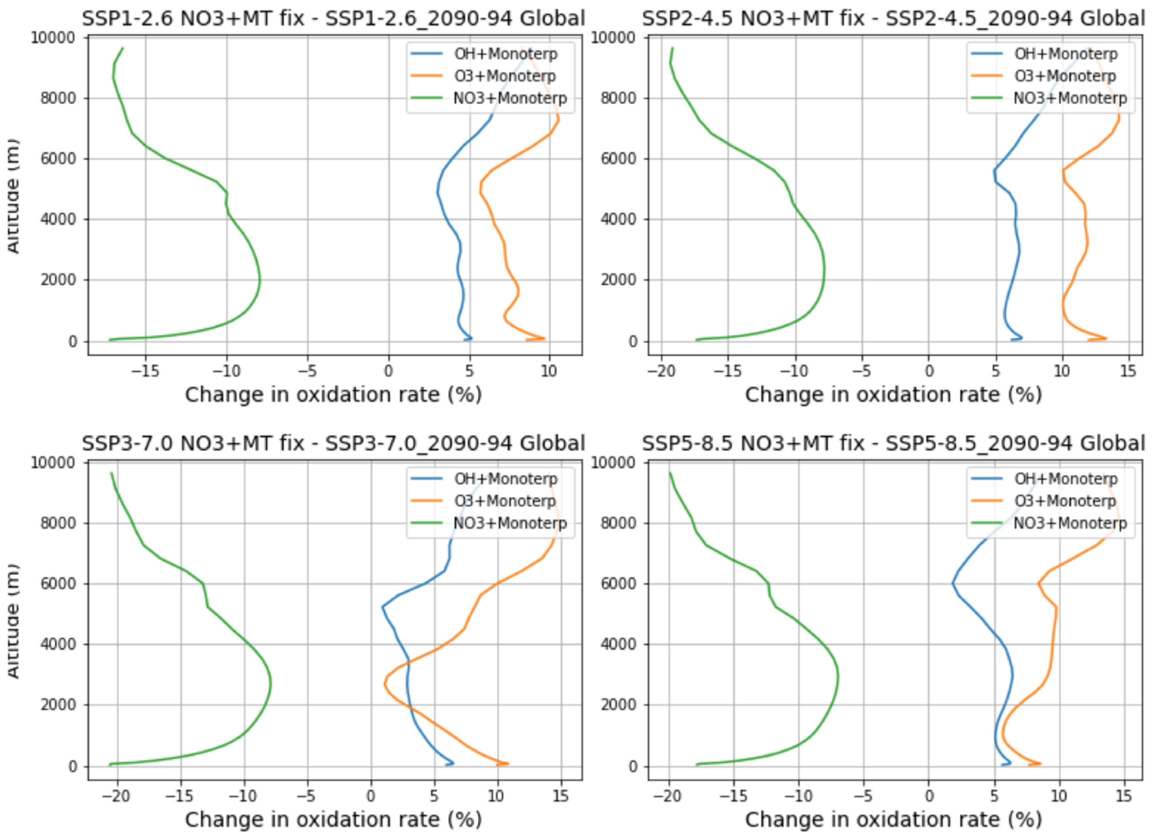

Fig. S2. Changes in global average oxidation rate between simulations with correction to NO3+Monoterpene reaction rate coefficient.

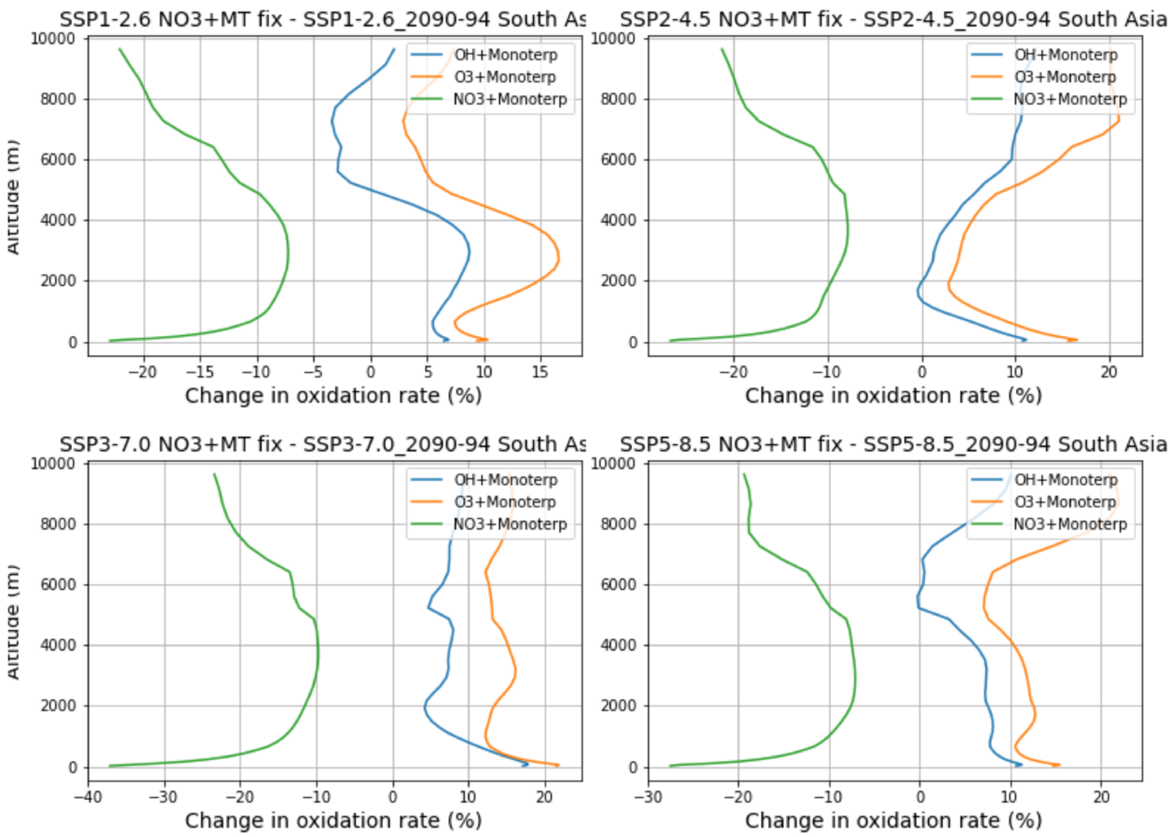

Fig. S3. Changes in oxidation rate averaged over South Asia region between simulations with correction to NO3+Monoterpene reaction rate coefficient.

Oxidation fluxes over other TF-HTAP regions

Figure S4 shows oxidation rate fluxes through the HTAP North America and East Asia regions, to complement Figure 4 in the main paper. Figure S5 shows oxidation rate in the vertical column for the present day and for each of the future model scenarios over the whole world, North America, South Asia and East Asia regions to complement Figure 5 in the main paper.

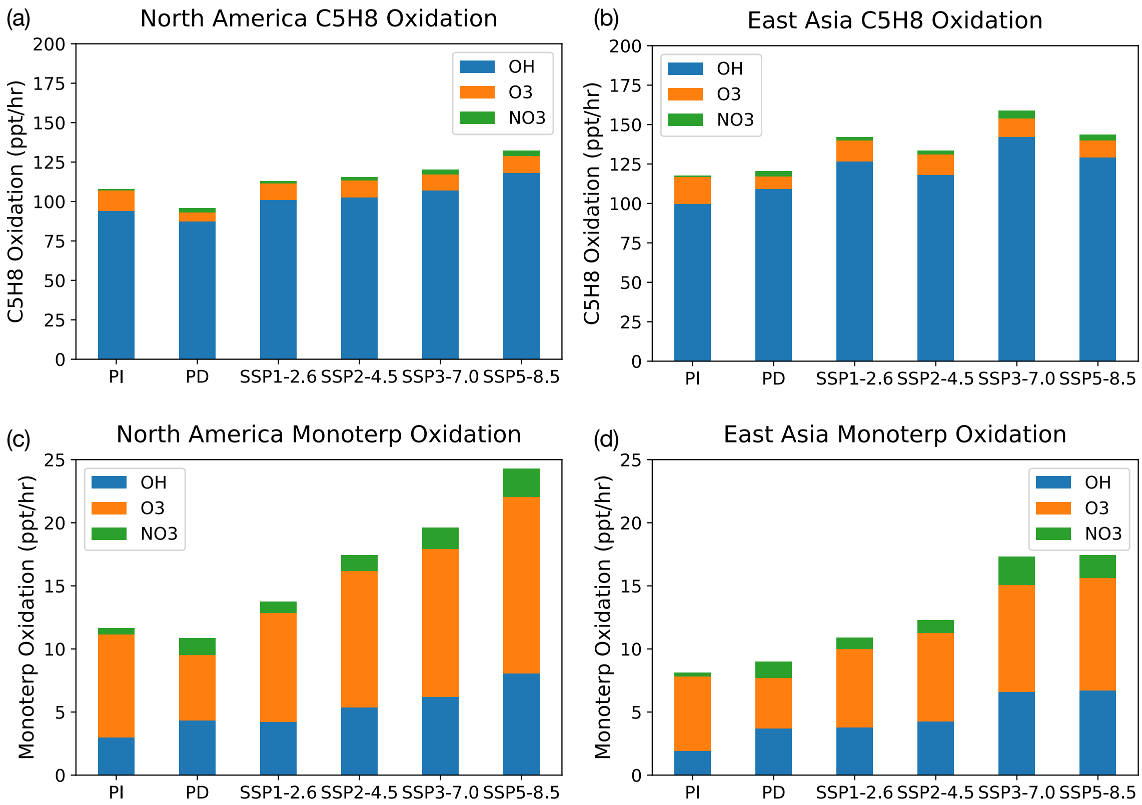

Fig. S4. Average oxidation rates in lower 1km of atmosphere for isoprene (a and b) and MONOTERP (c and d), averaged across the North America (a, c) and over East Asia (b, d) region.

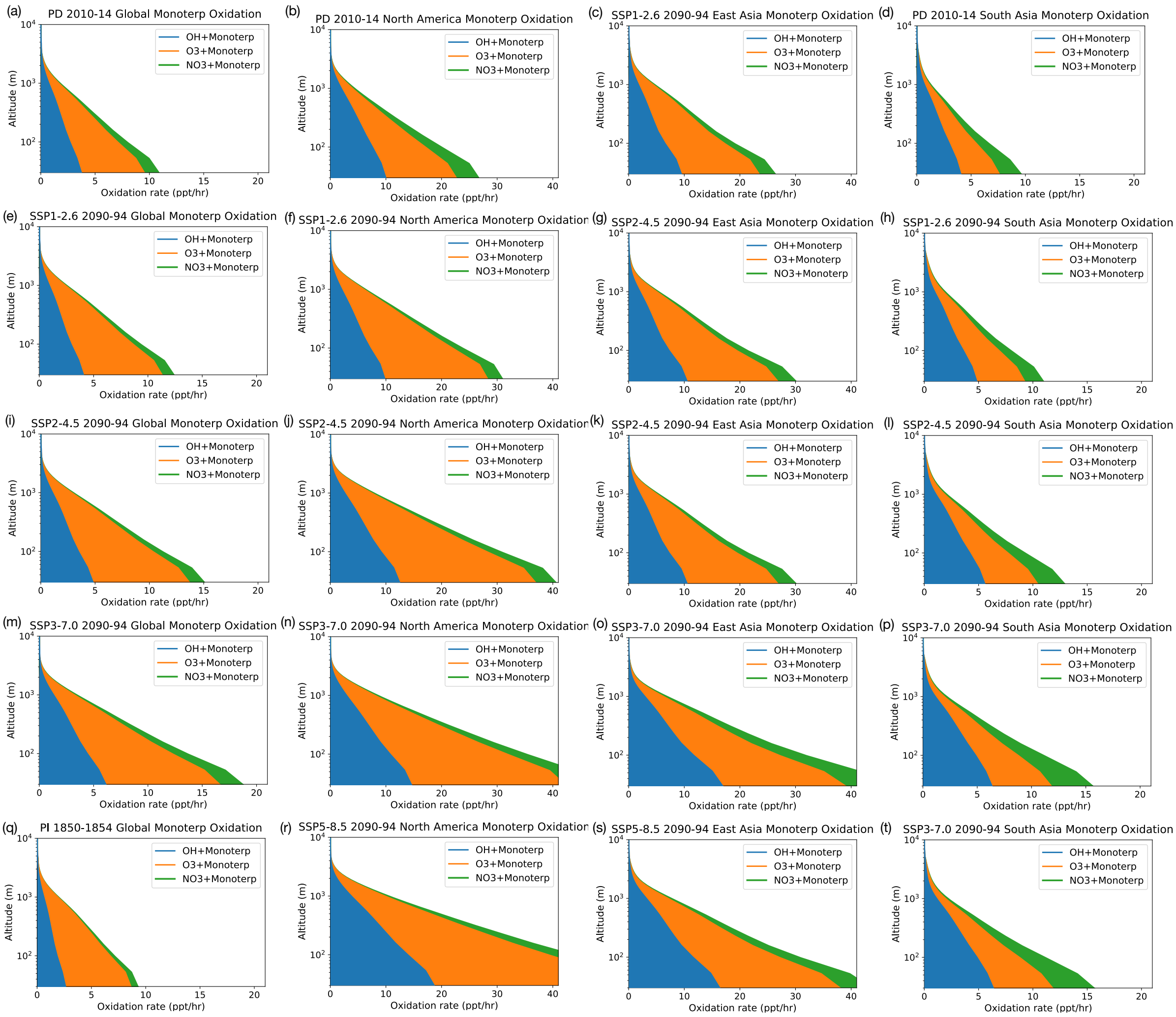

Fig. S5. Vertical profiles of MONOTERP oxidation via OH, O_3 and NO_3. Panels (a-d) are for PD conditions, (e-h) for SSP1-2.6 conditions in 2090-94, (i-l) for SSP2-4.5, (m-p) for SSP3-7.0 and (q-t) for SSP5-8.5. Columns from left to right show oxidation rates averaged over Global, North America, East Asia and South Asia regions.

S2. Table of additional simulations performed

Table S1. UM Rose suite information and branch information for the extra simulations with the corrected rate constant for NO_3+Monoterp. Processed netCDF data is available through CEDA. See Data Availability section in the Main Paper.

Experiment ID	Suite info	Branch info	Description
u-bz750	u-bl107@125788	vn11.2_no3_diag@91119	StratTrop with extra NO_3 diagnostics and correction to NO_3+Monoterp reaction rate, 2090-2094, SSP126
u-bz751	u-bl110	vn11.2_no3_diag@91119	StratTrop with extra NO_3 diagnostics and correction to NO_3+Monoterp reaction rate, 2090-2094, SSP245

u-bz752	u-bl123	vn11.2_no3_diag@91119	StratTrop with extra NO_3 diagnostics and correction to NO_3+Monoterp reaction rate, 2090-2094, SSP370
u-bz753	u-bl126@125793	vn11.2_no3_diag@91119	StratTrop with extra NO_3 diagnostics and correction to NO_3+Monoterp reaction rate, 2090-2094, SSP585
u-bz754	u-bl077@125529	vn11.2_no3_diag@91119	StratTrop with extra NO_3 diagnostics and correction to NO_3+Monoterp reaction rate, PI 1850-1854, Historical