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The TOMCAT global chemical transport model v1.6: description of chemical mechanism and model evaluation

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Supplementary Material for "The TOMCAT global chemical transport model: Description of chemical mechanism and model evaluation" by Monks et al.

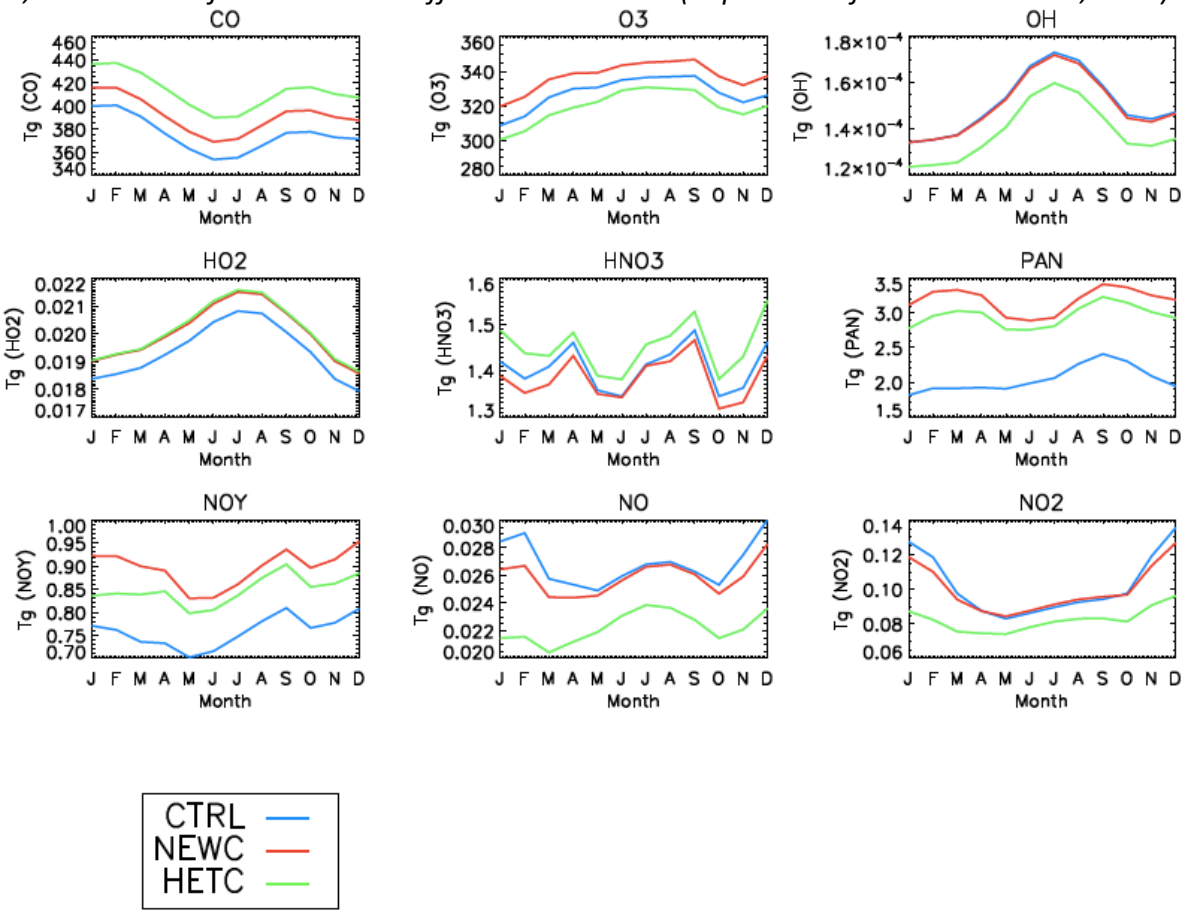
In order to demonstrate the impact of using the extended chemistry scheme (ExTC) and monoterpene chemistry in TOMCAT over the older version of the TOMCAT chemistry model used by Arnold et al. (2005) and Young et al. (2007) some results from Monks et al. (2011) are reproduced here. Monks et al., (2011) implemented the ExTC and monoterpene tropospheric chemistry scheme within an older version of the model. The main differences between this version and the current version of the TOMCAT model presented in the main body of this paper is that the current version of TOMCAT uses updated photolysis cross-sections and quantum yields, has corrected coding errors that led to errors in emissions, uses different emission datasets and improvements have been made to the model code that led to a more efficient model in terms of computational cost. The main purpose of the supplementary material is to simply demonstrate the change that occurred when the tropospheric chemistry was extended to include the ethene, propene, toluene, butane and monoterpene chemistry as described in Section 2.1 (referred to as NEWC) and when it was further extended to include uptake of N_2O_5 by aerosol, which is also described in Section 2.1 of the main paper (referred to as HETC). The simulations that have been taken from Monks et al. (2011) are summarized in Table S1.

The global monthly mass burdens from each of the simulations have been calculated for CO, O_3, HOx, HNO_3, PAN, NOy and NOx and are shown in Figure S1. CO is increased by 14-18 Tg (4-5 %) when the more detailed chemistry scheme is used (difference between the CTRL and NEWC simulations) due to enhanced secondary production of CO from the oxidation of the additional non-methane hydrocarbons (NMHC). The additional NMHC and CO lead to more O_3 production with the burden being 8-11 Tg (2-4 %) larger in NEWC compared to CTRL. The total mass burden of OH does not seem to be largely affected, but OH does show a 1% reduction in NEWC in summer due to reaction with the additional hydrocarbons and CO. Conversely, HO2 is increased by 3-4% due to the oxidation pathways of the additional hydrocarbons resulting in more formaldehyde and HO_2 production. One of the most significant changes is seen in PAN, where the burden is increased by 40-75%, with the biggest increase occurring during the NH winter when thermal decomposition of PAN is slower due to the lower temperatures. This large increase in PAN is due to an increase in the number of pathways that produce precursors of PAN. Thermal decomposition of the additional PAN in NEWC is likely to explain the increase in NO_2 in summer when temperatures are warmer in the NH. This could also be contributing to the increase in O_3 in the model. When the heterogeneous uptake of N_2O_5 by aerosol is also included in HETC, NOx is affected quite significantly, with NO and NO_2 decreasing by 10-20% and 10-27%, respectively (HETC compared to NEWC). The biggest change occurs in January and February during dark conditions and low temperatures when loss of N_2O_5 is most efficient. This results in an increase in HNO_3 and a decrease in PAN. As the formation of HNO_3 acts as a sink of NOx from the atmosphere, overall, NOy is reduced by up to 10% in winter. As NOx is important for O_3 production, the burden of O3 decreases by 4-6%. As OH is formed from the photolysis of O_3, the burden of OH is also lowered by 7-8%. Due to a smaller global OH burden, CO has a longer lifetime increasing the global burden by 5-6%.

Table S1. The three simulations discussed in the supplementary material.

Simulation ID	Description	Emissions
CTRL	Control simulation	AR5 anthropogenic emissions, POET natural emissions, GFED v2 2008 biomass burning emissions.
NEWC	Additional hydrocarbon and monoterpene emissions and chemistry.	AR5 anthropogenic emissions, POET natural emissions, GFED v2 2008 biomass burning emissions.
HETC	Same as NEWC but with heterogeneous uptake of N_2O_5 on black carbon, organic carbon, dust, sulphate and sea-salt. (dust $\gamma = 0.02$).	AR5 anthropogenic emissions, POET natural emissions, GFED v2 2008 biomass burning emissions.

Figure S1. The global monthly mean tropospheric burdens of CO, O3, OH, HO2, HNO3, PAN, NOY, NO and NO2 from the three different simulations (Reproduced from Monks et al., 2011).



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