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Modelling trends in OH radical concentrations using generalized additive models

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Abstract. During the TORCH campaign a zero dimensional box model based on the Master Chemical Mechanism was used to model concentrations of OH radicals. The model provided a close overall fit to measured concentrations but with some significant deviations. In this research, an approach was established for applying Generalized Additive Models (GAM) to atmospheric concentration data. Two GAM models were fitted to OH radical concentrations using TORCH data, the first using measured OH data and the second using MCM model results. GAM models with five smooth functions provided a close fit to the data with 78% of the deviance explained for measured OH and 83% for modelled OH. The GAM model for measured OH produced substantially better predictions of OH concentrations than the original MCM model results. The diurnal profile of OH concentration was reproduced and the predicted mean diurnal OH concentration was only 0.2% less than the measured concentration compared to 16.3% over-estimation by the MCM model. Photolysis reactions were identified as most important in explaining concentrations of OH. The GAM models combined both primary and secondary pollutants and also anthropogenic and biogenic species to explain changes in OH concentrations. Differences identified in the dependencies of modelled and measured OH concentrations, particularly for aromatic and biogenic species, may help to understand why the MCM model predictions sometimes disagree with measurements of atmospheric species.

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