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Comparisons of observed and modeled OH and HO_2 concentrations during the ambient measurement period of the HO_xComp field campaign

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A photochemical box model constrained by ancillary observations was used to simulate OH and HO_2 concentrations for three days of ambient observations during the HO_xComp field campaign held in Jülich, Germany in July 2005. Daytime OH levels observed by four instruments were fairly well reproduced to within 33% by a base model run (Regional Atmospheric Chemistry Mechanism with updated isoprene chemistry adapted from Master Chemical Mechanism ver. 3.1) with high R2 values (0.72-0.97) over a range of isoprene (0.3-2 ppb) and NO (0.1-10 ppb) mixing ratios. Daytime HO_2(*) levels, reconstructed from the base model results taking into account the sensitivity toward speciated RO_2 (organic peroxy) radicals, as recently reported from one of the participating instruments in the HO_2 measurement mode, were 93% higher than the observations made by the single instrument. Adding isomerization of isoprene peroxy radicals to the model increased OH and HO_2(*) by 28% and 13% on average. Although these are still only 4% higher than the OH observations made by one of the instruments, larger overestimations (42-70%) occurred with respect to the OH observations made by the other three instruments. These model runs tend to underestimate observed OH reactivity which may be explained by unmeasured hydrocarbon species. In the base run, the good agreement for the OH levels was retained when four different types of hydrocarbons were added as mixture to explain the missing OH reactivity. In the model run with isomerization of isoprene peroxy radicals, on the other hand, OH levels agreed to the ensemble of observations only when unmeasured anthropogenic hydrocarbons was added at implausibly high concentrations, implying that the rates of the isomerization were not readily supported by the ensemble of radical observations. The overprediction of the HO_2(*) levels by the model occurred independently of the inclusion of the isoprene isomerization scheme, indicating that more loss processes for peroxy radicals were necessary to explain the observations. One of the measurement days was characterized by low isoprene concentrations ($\sim$0.5 ppb) and OH reactivity that was well explained by the observed species, especially before noon. For this selected period, as opposed to the general behavior, the model tended to underestimate HO_2(*). We found that this tendency is associated with high NO_x concentrations, suggesting that some HO_2 production or regeneration processes under high NO_x conditions were being overlooked; this might require revision of ozone production regimes.