Elevated levels of OH observed in haze events during wintertime in central Beijing

Supplementary Information

The MCM-base model, which uses a deposition rate of 0.1/MH, has been run again using several different deposition rates for the model generated intermediates. The effect of changing the deposition rate on the concentration of OH, HO_2 and RO_2, and also on the OH reactivity, kOH, is shown in Figure S1. Figure S1 shows that changing the deposition rate does not change the radical concentration significantly (less than 5%), and for the OH reactivity the maximum difference is 10%. The small changes in OH reactivity when the deposition rate is changed by a factor of 10 shows that the model intermediates do not contribute significantly to the OH reactivity, rather the OH reactivity is dominated by measured, primary emissions. It also shows that the deposition rate used in the MCM-base model run is appropriate as the OH reactivity is replicated well, and changes in the deposition rate do not change the total radical concentration significantly.

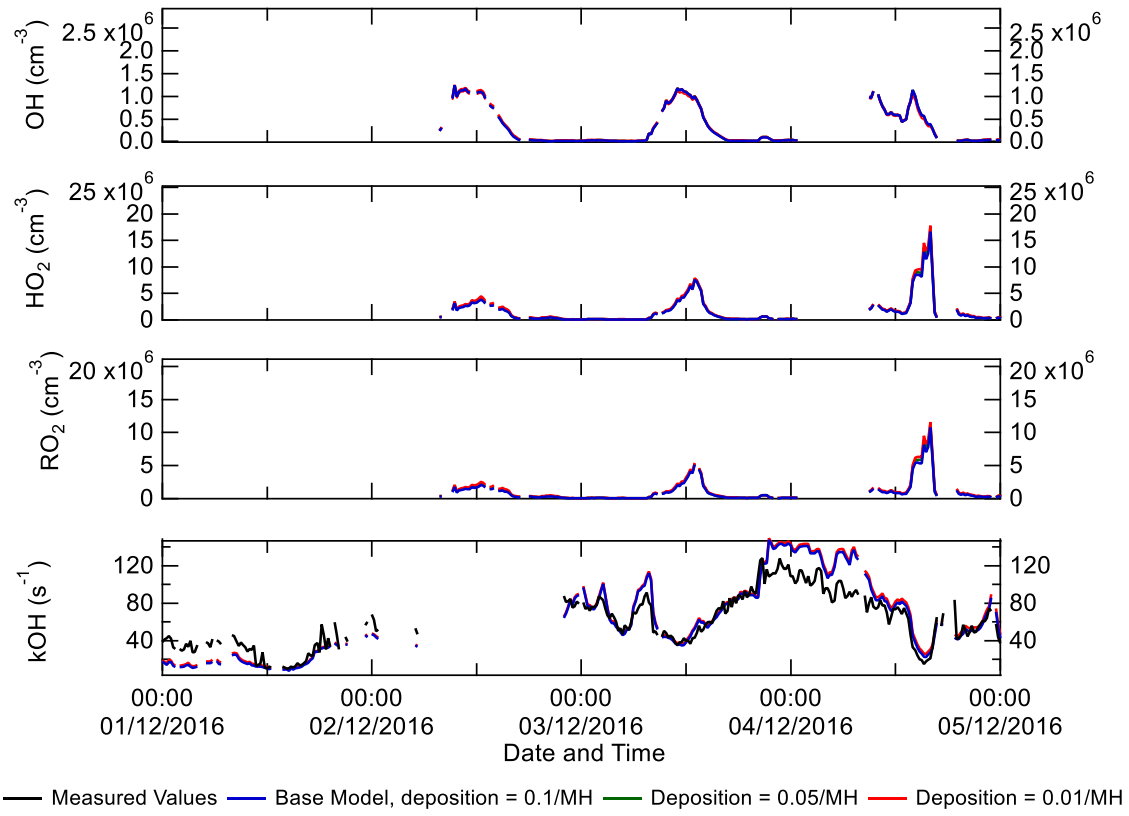

Figure S1. Effect of changing the deposition rate for model generated intermediates on the concentrations of OH, HO_2 and RO_2, and the OH reactivity, together with a comparison with the measurements.

For the winter campaign only, VOC species up to C7 were measured by the DC-GC-FID, but to test the sensitivity of the model to higher weight VOCs, measurements from a PTR-MS were incorporated into the MCM-base model to include C2 and C3 aromatic species. The species measured by the PTR-MS and used in this model run, MCM-fVOC, were ethyl benzene(C2), propyl benzene(C3), isopropyl benzene(C3), 2-Ethyltoluene(C3), 3-Ethyltoluene(C3), 4-Ethyltoluene(C3), 1,3,5-trimethylbenzene(C3), 1,2,4-trimethylbenzene(C3) and 1,2,3-trimethylbenzene (C3). Since the DC-GC-FID measured three C2 aromatic species (o-xylene, m-xylene and p-xylene) the concentration of ethyl benzene was calculated through the difference between the PTR C2 and the DC-GC-FID C2 measurements. The model comparison between MCM-base and MCM-fVOC model runs is shown in Figure S2, and shows that introducing higher weight VOCs does not effect the radical concentration significantly, with the largest difference observed on the 5/12/2016 of ~7%.

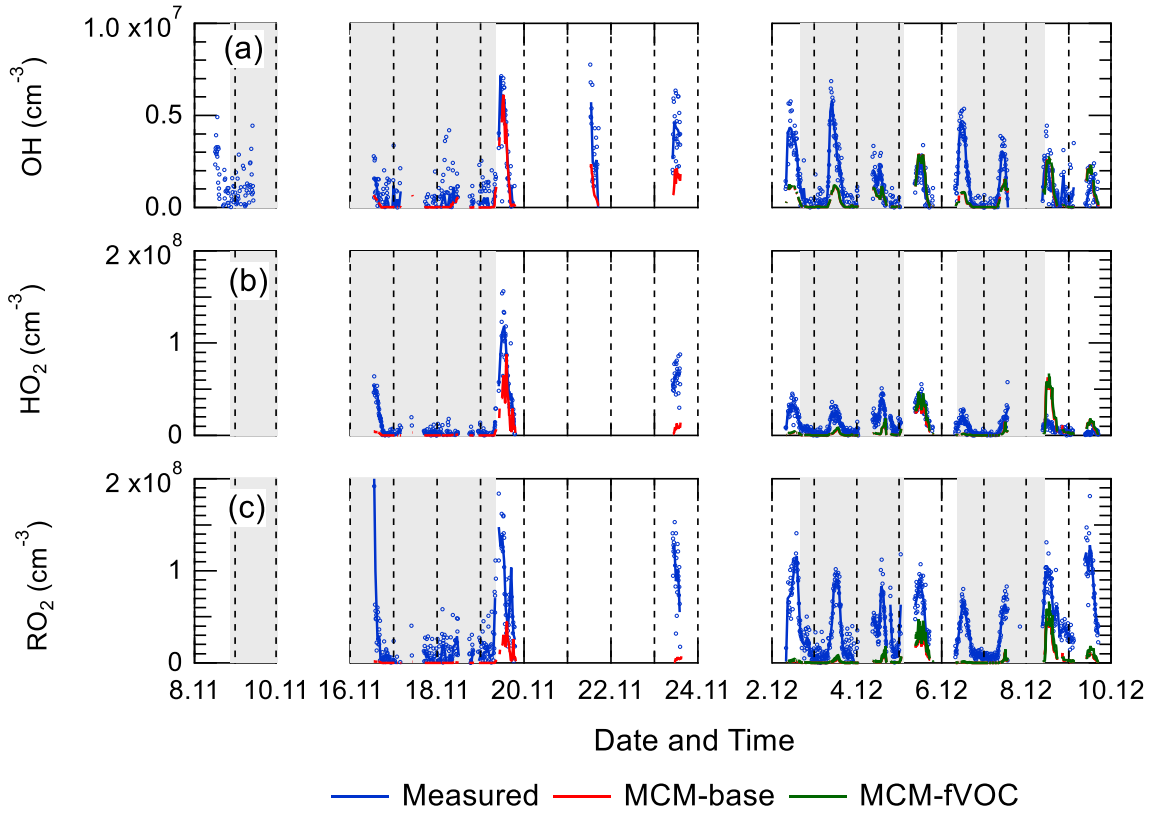

Figure S2 a) Comparison of measured OH with modelled OH from MCM-base and MCM-fVOC. b) Comparison of measured HO_2 with modelled HO_2 from MCM-base and MCM-fVOC. c) Comparison of measured total RO_2 with modelled total RO_2 from MCM-base and MCM-fVOC. It should be noted that PTR-MS data were only available from 24/11/2016 onwards, hence the data comparison is only between the 02/12/2016 – 10/12/2016.

The impact of the higher weight VOCs in the model on OH reactivity is shown in Figure S3, and shows that introducing the higher weight VOCs has a very small impact on modelled kOH,

Also the modelled kOH from the MCM-fVOC model run is in good agreement with measured kOH. These results show that the MCM-base model does not have a large sensitivity to the introduction of higher weight aromatic species.

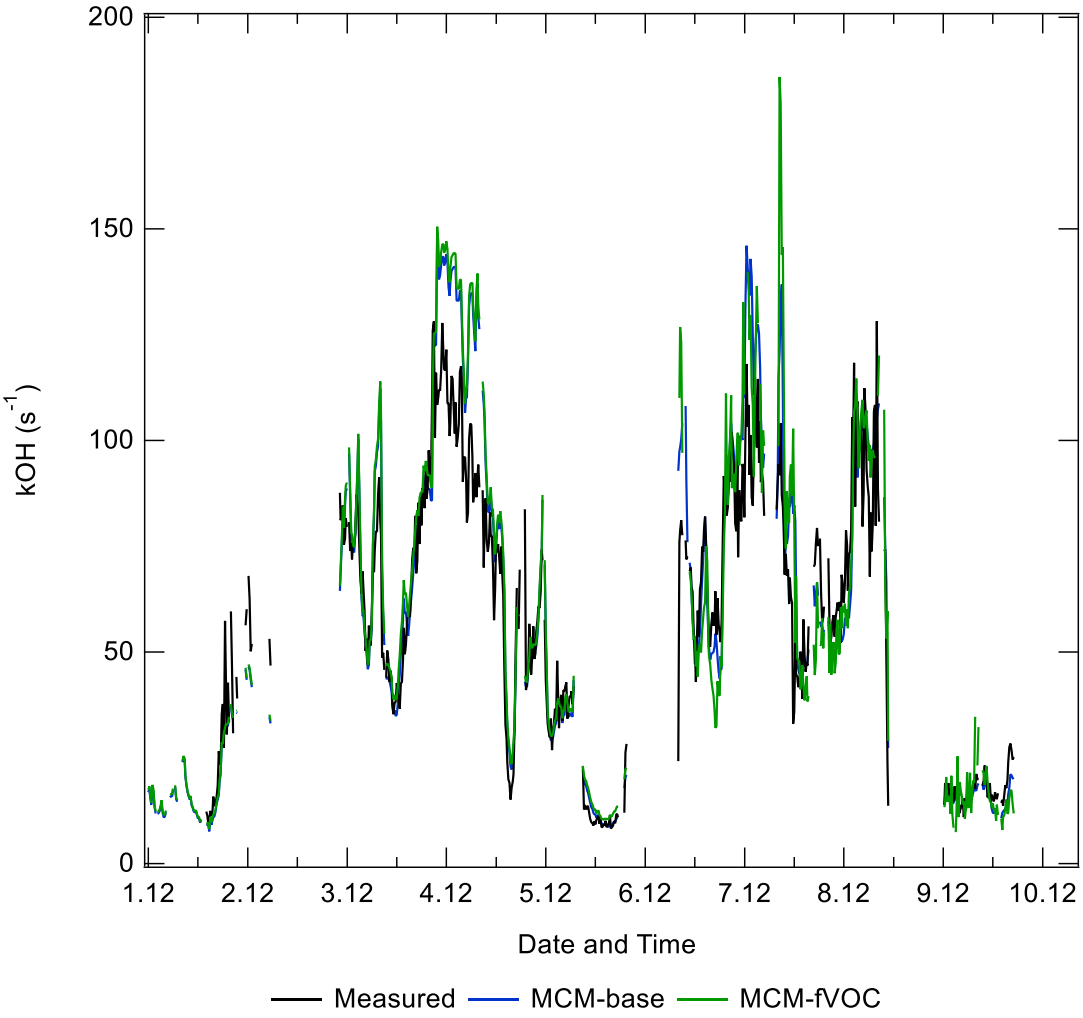

Figure S3 Comparison of measured OH reactivity (kOH) with modelled OH reactivity from the model runs MCM-base and MCM-fVOC.