Supplement of Atmos. Chem. Phys., 21, 2125–2147, 2021
https://doi.org/10.5194/acp-21-2125-2021-supplement

Atmospheric Chemistry and Physics
Open Access
EGU

Supplement of

Evaluating the sensitivity of radical chemistry and ozone formation to ambient VOCs and NO_x in Beijing

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Supplementary Information

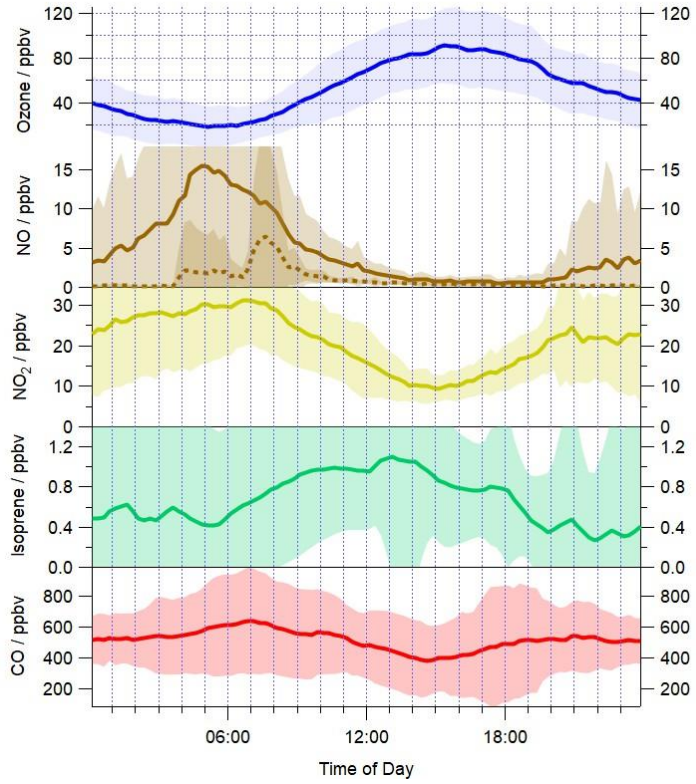

Figure S1: Average profiles for the observed O_3, NO, NO_2, isoprene, and CO at 15 minute intervals over 24 hours. The solid lines represent the campaign average whilst the dashed line is the average NO profile between 16th – 22nd June.

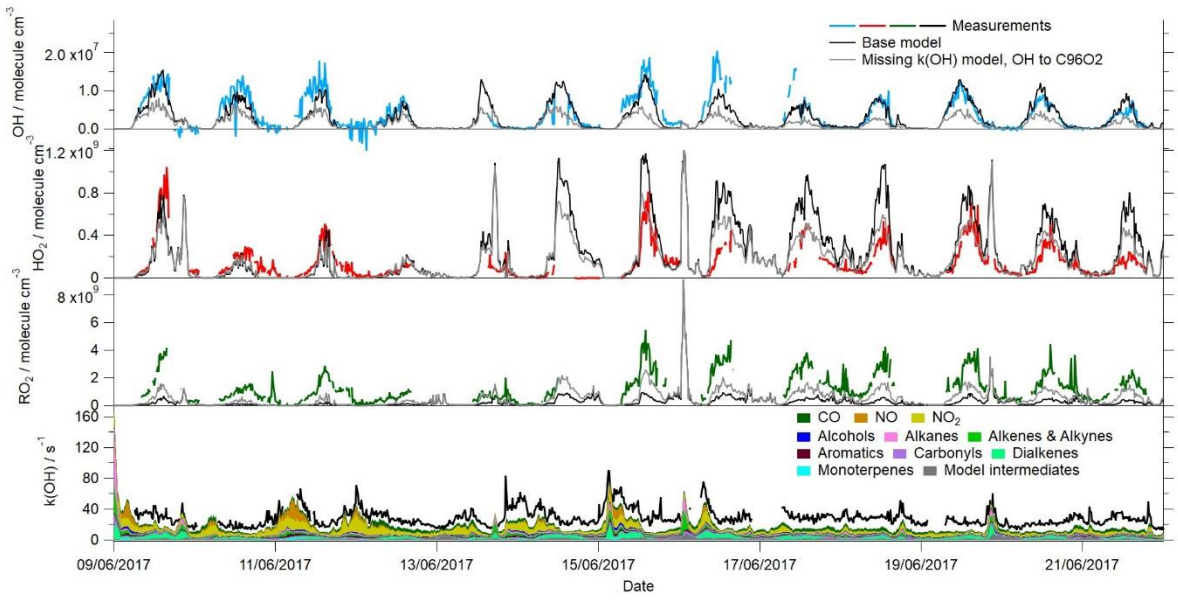

Figure S2: Time-series of the measured and modelled OH, HO_2, total RO_2 and OH reactivity from the 9th – 22nd June which encompasses high NO days (9th – 12th June) and low NO days (16th – 22nd June).

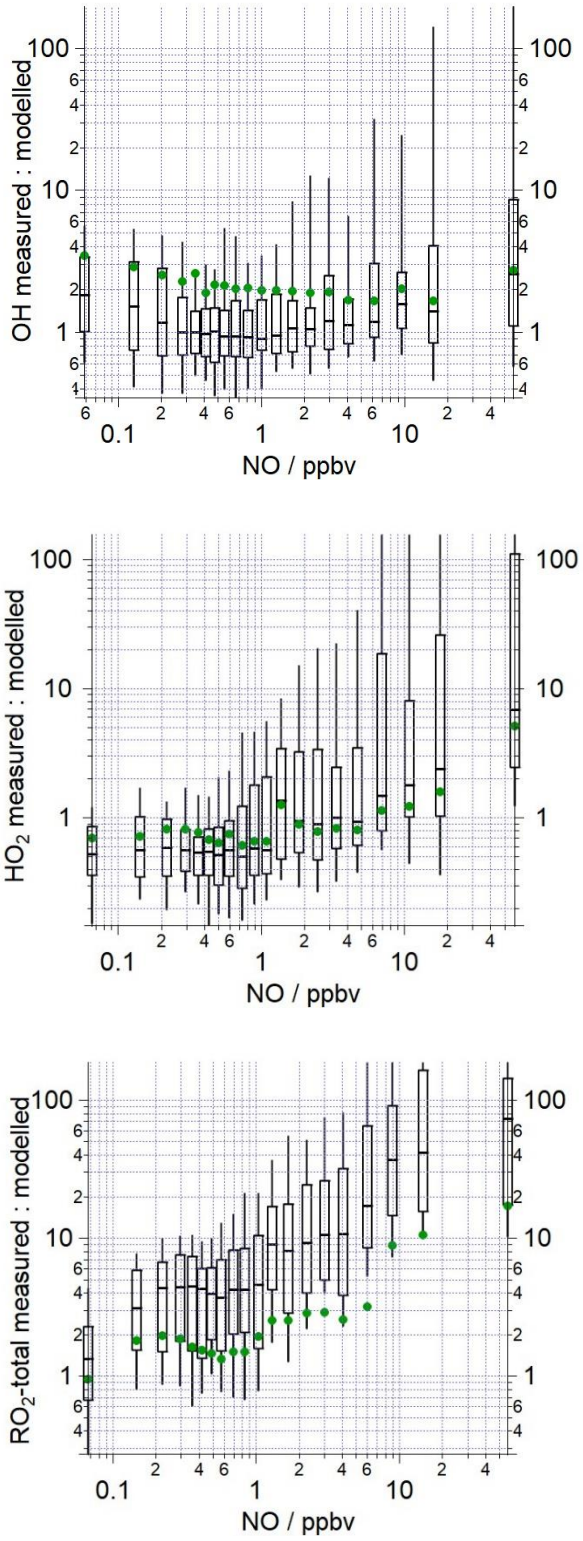

Figure S3: The median ratio (-) of the measured to modelled (base) OH, HO_2 and total RO_2 binned over the NO mixing ratio range encountered during the campaign on a logarithmic scale. The box and whiskers represent the 25th/75th and 5th/95th confidence intervals. The green circles display the measured to modelled OH, HO_2 and total RO_2 ratio when the model includes missing OH reactivity in the form of a single reaction which converts OH to C96O2. The number of data points in each of the NO bins is ~80.

The median measured to modelled (Missing k(OH) (OH to C96O2)) ratio vs NO (green circles) is displayed in figure S3 alongside median measured to modelled (base) ratio. The inclusion of alkoxy isomerisation following RO_2 + NO reaction increases the modelled RO_2 concentration across the entire NO range (bottom panel) but, considering the log scale, has the biggest impact on the ratio (from the measured to modelled (base) ratio) at the highest NO concentration. The HO_2 median measured to modelled (Missing k(OH) (OH to C96O2)) ratio vs NO in the middle panel increases from the measured to modelled (base) ratio at NO mixing ratios <1 ppbv, indicating improved agreement. At higher NO mixing ratios, where the base model begins to underpredict HO_2, due to the large under-prediction in RO_2, this under-prediction is reduced in the missing k(OH) (OH to C96O2) scenario owing to the increase in modelled RO_2.

The HO_2 median measured to modelled (Missing k(OH) (OH to C96O2)) ratio vs NO in the middle panel increases from the measured to modelled (base) ratio at NO mixing ratios <1 ppbv, indicating improved agreement. At higher NO mixing ratios, where the base model begins to underpredict HO2, due to the large under-prediction in RO_2, this under-prediction is reduced in the missing k(OH) (OH to C96O2) scenario owing to the increase in modelled RO_2.

The OH median measured to modelled (Missing k(OH) (OH to C96O2)) ratio vs NO (top panel) highlights a missing OH source, the magnitude of which deceases as NO concentrations increase.