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Comment on acp-2021-44

Anonymous Referee #1

Referee comment on "Development of ozone reactivity scales for volatile organic compounds in a Chinese megacity" by Yingnan Zhang et al., Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2021-44-RC1, 2021

Development of Ozone Reactivity Scales for Volatile Organic Compounds in a Chinese Megacity

ACP-2021-44

Zhang, Xue, Carter, Pei, Chen, Mu, Wang, Zhang and Wang

Zhang et al. describe a comprehensive analysis of reactivity scales for a Chinese megacity, Guangzhou. They use two methods to characterise base conditions for their Master Chemical Mechanism (MCM) box model. In one, model inputs are based on observations and in the other they are based on emissions. Four reactivity scales were determined using base conditions, maximum incremental reactivity (MIR), maximum ozone reactivity (MOR) and equal benefit incremental reactivity (EBIR) conditions. MOR and MIR reactivity scales estimated for Guangzhou were compared with the corresponding scales for USA conditions using the same chemical mechanism and with the SAPRC-07 mechanism. Sensitivity tests were performed to investigate the influence of environmental conditions on the estimated reactivity scales.

This is a comprehensive study which is well worth publishing in ACP. It should provide the essential data required in the formulation of strategies for tackling elevated ozone levels across China. I particularly liked Figure 2 and how the study links the MIR scale to VOC-limited conditions, MOR to mixed and EBIR to NO_x-limited conditions.

The study fulfils an important service in providing in Table 1 the IRs for all 116 VOC species in the MCM under the four sets of conditions. Elsewhere in the study more use should be made of relative incremental reactivities, by expressing them relative to a

specific VOC such as ethene. Zhang et al. introduce the concept as MIR/Ethene though much more use could be made than the brief mention in section 3.2 (lines 227 onwards). The advantage of relative reactivities is that they clearly reveal small differences between reactivity scales. When discussing the influence of background conditions (lines 270 onwards), these would be much clearer if they were presented as ratios to ethene: IRs/IR_{ethene}. Table 2 should be replaced with Tables of IR/IR_{ethene} values then we could see if the background conditions really changed the reactivities for particular VOCs. Also, in Figures 5 and 6, we see the differences in reactivity scales between Guangzhou and USA. But these would be much more illuminating if they were presented as IR/IR_{ethene} values rather than as ranks. Ranks disguise the magnitudes of the differences.

In reading through the preprint, some trivial issues were noted.

- line 30: Agathokleous et al. is not the best reference to give here. There is an excellent reference available from the Tropospheric Ozone Assessment Report in Elementa.
- line 47: What is meant here? A mechanism is either explicit or not. If it contains non-stoichiometric chemical equations then it is not explicit.
- line 72: 'results obtained'.
- lines 86-87: It is widely recognised that the diurnal cycle in ozone is caused by changes in the stability of the boundary layer and not by intense in situ photochemical ozone production. This is explained in the Tropospheric Ozone Assessment Report.
- line 93: ppbv $ppbv^{-1}$.
- line 99: Reference to the MCM website at the University of York would be more up-to-date.
- line 112: Where does these initial concentrations come from if not from observations? There are many sets of OVOC data for China.
- line 128: Replace 'folds' with scaling factors.
- line 134 onwards: please explain what the 'base' scenario is.
- line 176: The chemspider website reference provides rate coefficients presumably and not reaction fluxes.
- line 238-242: It would be exceptionally useful if a little more detail was given here about why the five outliers are difficult to represent in chemical mechanisms. Benzene and styrene, presumably like phenol, are strong inhibitors of ozone formation. Is there a simple explanation how this works mechanistically. Then we have n-octane through n-decane. Presumably the mechanism of inhibition is different here and it would be interesting to know why this is. Why does it begin with n-octane and not n-heptane?
- line 241: This point would be self-evident if the presentation had been done with MIR/MIR_{ethene} ratios.
- line 244: MIR
- line 250: What was done with one quarter of the base ratios?
- Section 3.2: This is a big section that would benefit considerably from being split into smaller sub-sections.
- line 336 onwards. This is an important recommendation and should be in the Conclusions section with a little more explanation.