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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Observationally constrained modelling of atmospheric oxidation capacity and photochemical reactivity in Shanghai, China" *by* Jian Zhu et al.

Anonymous Referee #2

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General Comments

This paper presents a set of recent (2018) measurements of trace gases from a ground site in Shanghai to assess the factors that lead to photochemical ozone pollution in that region of China. The measurements span five months of nearly continuous measurements. They include NOx and speciated VOCs, among other chemical measurements, together with standard meteorological data (but not including boundary layer dynamics).

The results are analyzed in the context of three different case studies of high, medium and low ozone. Several different standard metrics of photochemistry and ozone pro-

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duction are used to analyze the data using both observationally derived quantities as well as box modeling.

While the overall measurements and analysis are standard and do not present any novel data or analysis methods, they do represent a comprehensive analysis from a particular year and location in China, a highly polluted region that is currently undergoing a transition from recent high emissions to somewhat lower and more controlled emissions of common air pollutants. They will therefore represent a useful data point and analysis of factors that control ozone pollution in a Chinese megacity.

The manuscript is generally well written and easy to follow.

I recommend publication following attention to the minor comments and technical corrections below.

Minor Comments

Line 21, Abstract: AQI is not defined here nor referenced further in the text. The wording is also not clear. 92.2% of all the days in the observation period ? Or some fraction of the AQI ?

Line 34, Abstract: "Concentration ratio" should be defined. This is the summed mixing ratio of these species relative to what? Total NMVOC? Or total carbon ? Also, the statement that follows implies that these four compounds could be controlled, but since HCHO is not a direct emission, it would result from control of all VOC and could not be targeted individually.

Line 73: The differences described are not all a function of metropolitan areas but also of the season in which the measurements took place. The Ren 2003 reference, for example, was in winter, one of the main reasons that HONO photolysis is listed as important. The list is also not a comprehensive literature review, which should be stated, as there are numerous similar analyses in addition to those listed here.

Line 89: Remove "the of". What does the growth rate refer to ? Average O3? Maximum

O3 ? Number of air quality exceedances ?

Line 125: Define “ultra-low temperature”

Line 141: PAN is not technically defined as an oxidant, but is co-produced with O3.

Line 145-146: The model procedure is not clear. A seven-day run is constrained to data throughout, with seven days of continuous measurements? Or is the run constrained to some sort of diel average? Why does it require four days to reach a steady state? Which species require this spin up time?

Line 150, AOC: The definition of AOC does not include NOx, notably not the reaction of OH with NO2, but also not RO2 + NO reactions (i.e., producing organic nitrates). These are chain termination steps and so perhaps are excluded for that reason, but the exclusion would not then fit the definition that follows of defining the “removal rate of most pollutants”, since NOx (as well as SOx) is excluded. Some comment or caveat to this effect is warranted, even if the definition is simply following prior literature. The quantity as defined is not as commonly used as other metrics in this paper.

Line 162, OH chain length: This is one of several available definitions. The assumption in this formulation appears to be that OH + NO2 is the major chain termination reaction. This is shown in the later analysis but not justified here. The later analysis needs to be referenced to justify this equation. In some instances, RO2 + NO producing organic nitrates is competitive with OH + NO2. No mention is made of this chain termination step, nor is its importance ever assessed in the context of other metrics. This chain termination reaction needs to be included in the metrics of ozone photochemistry somewhere in this paper.

Line 191-192: Is radiation the only factor ? From Figure 1, it appears that meteorology and transport could also easily have been important. The temperature, relative humidity, and distribution of wind vectors were also different between the two periods.

Line 212: Acetylene is not technically an alkene but rather an alkyne. It is much less

reactive than alkenes towards OH. This is described in footnote c of table 2, but would be better also in the text. The lumping of acetylene with alkenes is not really appropriate, but if it is done, the statement that this compounds is far less reactive with alkenes toward OH needs to be explicit.

Line 215, Table 2: Units are given in footnote (b) but are otherwise difficult to find. Suggest moving this description to the table caption.

Line 229-230, and 235-239: Were there NO3 measurements to define nighttime AOC ? The NO3 measurement (by DOAS ?) is not specified in the experimental techniques. Was this a calculated quantity ? Was there nighttime NO at the surface level measurement site that limited NO3 ?

Line 238: Numbers given for NO3 do not match the figure, which always shows much larger AOC due to OH. Do these percentages refer to nighttime data only ?

Line 310: Clarify what is meant by "all within 10". This could imply a factor of 10 difference between chain lengths, which is likely not what is intended.

Line 312: This is not "probably" due to higher NOx, but rather simply "due to higher NOx", correct? The dependence should not be difficult to infer.

Line 313-315: The OH chain length is described at the beginning of the paragraph as being similar to ozone production efficiency, yet here trend in OH chain length is show to be opposite to ozone abundance. Can the authors reconcile these statements?

Line 344-350: The photolysis of ClNO2 was noted in an earlier section and should be noted here again as previous studies have shown it to be as important as HONO during the morning hours (e.g., Young, ES&T, v 46, p10965, 2012)

Line 367: Where do the calculated MIR coefficients come from in this equation? How are they determined ?

Line 412-414: Same comment as in the abstract. While three of the four NMVOC can

in fact be controlled, formaldehyde is mainly the secondary oxidation product from a wide range of other compounds and cannot be controlled directly.

Technical Corrections

Line 23, Abstract: The word “premise” is not properly used here.

Line 32, Abstract: “radical” rather than “radicals”

Line 83: Replace “even more” with “increasingly”; Line 86: remove the word “around”

Line 104, 123, 153, 336, 409: Replace “Besides” with “Additionally”

Line 143: “input” rather than “inputted”

Line 170: Pollutants shown in Figure 1 are given in mixing ratio, not concentration units.

Line 223: “based” rather than “base”

Line 289: Eliminate the word “besides”

Line 373: Figure gives mixing ratios rather than concentrations. Specify mixing ratio in text.

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