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Geoscientific Model Development Discussions

Interactive comment on "Global tropospheric effects of aromatic chemistry with the SAPRC-11 mechanism implemented in GEOS-Chem" *by* Yingying Yan et al.

Anonymous Referee #2

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This paper reported an excellent timely effort updating aromatic VOC chemistry in GEOS-Chem, a widely used global chemistry model. The effort is very useful for the community given the importance of aromatics in regional and global chemistry and the potential limitation of the existing chemical mechanism included in GEOS-Chem. The paper describes the motivation, methodology in a very clear fashion. The key model results (e.g., NOx, HOx, ozone) are selected appropriately and discussed thoroughly, and are interpreted carefully by recognizing both the strengths and the potential limitations of the model setup and input data. A very comprehensive model evaluation has been carried out using data from multiple global and regional networks/programs. I recommend publication after my following comments are considered.

Major comments

- The use of AQS ozone data in model evaluation is inappropriate and should be removed

It is simply inappropriate to directly compare urban and suburban AQS ozone observations near the surface ($\sim$ 10 m) to GEOS-Chem ozone at 65 m height with 2x2.5 deg horizontal resolution. The model evaluation results using AQS data is not only meaningless but also misleading, especially when these results are discussed along with other networks in remote environments, where the model evaluation is actually appropriate and meaningful. Thus, I strongly suggest the authors remove the model evaluation with AQS ozone and focus on using networks over rural and clean environments.

- The adoption of SAPRC-11 and uncertainties in knowledge of aromatic chemistry

The paper describes the SAPRC-11 mechanism itself in detail and the method to include it into GEOS-Chem clearly. However, it is yet to be more clear why it is chosen instead of other options, such as the condensed MCM mechanism. One thing about SAPRC is the use of maximum ozone formation as a primary metric in the chamber experiment benchmark, and the mechanism has been primarily used and evaluated in regional CTMs such as CMAQ and CAMx, at much finer resolution (i.e., a few kilometers). I think the present paper is the first to use it in a global model. Therefore, the authors should have some words justifying the approach. Also, are there other considerations behind the simplified GEOS-Chem aromatic chemistry, in addition to minimizing the number of reactions? Moreover, it should be noted that our knowledge about the very complex aromatic chemistry itself is not complete. For instance, how would the uncertainties in the yields of di-carbonyls and radical recycling affect the mechanism and the model simulations? The simplified chemistry in GEOS-Chem does not have radical cycling, but are there any assumptions/uncertainties in SAPRC-11 about radical cycling that might have impact on the results too?

Adding some discussions on these above questions would make the paper even stronger.

Minor comments

P2, L19-L21: “Despite the potentially important influence of aromatic compounds on global atmospheric chemistry, their effect on tropospheric ozone formation in polluted urban areas remains largely unknown.” “Unknown” is an overstatement of the issue to me. Aromatic VOCs have long been recognized as a key player in urban photochemistry, forming PAN and ozone, and SOA, despite the uncertainties with the chemistry (and emissions).

P2, L21-L22: “The main source and sink processes of tropospheric ozone are photochemical production and loss, respectively (Yan et al., 2016)” Other references such as textbook by Seinfeld and Pandis (2006) would be more appropriate in this sentence.

P2, L33: “. . . including the parameterization of small-scale processes and their feedbacks to global-scale chemistry (Yan et al., 2014; Yan et al., 2016).” Other references should be added in addition to these two.

P5, L27: “The OH-aromatic adduct is reaction with O2. . .” This sentence needs rephrase.

P6, L13: Have the authors considered evaluating species other than ozone and aromatics, such as aircraft measurements of HOx (CalNex probably has some HOx measurements)?

P7, L32: Data download link does not work (last access 9/26/18) http://aqsdr1.epa.gov/aqsweb/aqstmp/airdata/download_files.html

P7, L36: see my first major comment.

P12, L30: The discussions at AQS sites should be removed.

P13, Section 5.4: See my second major comment. I suggest adding discussions of un-

certainty in knowledge of aromatic chemistry and the considerations and assumptions in SAPRC-11.

Table 2: I suggest add numbers for NH and SH

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