

## **Interactive comment on “The atmospheric chemistry box model CAABA/MECCA-4.0gmdd”**

**by Rolf Sander et al.**

This paper by Sander et al., essentially provides a basic reference for updates and developments included in the update of the CAABA/MECCA atmospheric chemistry box modelling toolkit to version “4.0gmdd”. This includes (1) updates and extensions to the chemical mechanism (Mainz Organic Mechanism), including updated SARs and photolysis rates; (2) provision of a range of alternative chemical mechanisms; (3) provision of a chemical skeletal reduction tool; (4) provision of a range of submodels for the calculation of photolysis rates throughout the atmosphere and (5) provision of a range of tools in order to connect MECCA to other modelling frameworks, including the MESSy 3-D global model. A range of other minor changes are also listed. The complete updated code discussed is made available to the community through the electronic supplementary along with a useful user manual section.

Although this type of is important and extremely useful to the community as a reference and “one stop shop” for this version of the CAABA-MECCA model, I found the paper reads very much like a report, listing the work done, and is therefore very dry to read. The descriptions of the work are basic and not particularly informative as to what has been done and why, and the impact of the changes. At the moment, the paper is only really useful to an experienced user of the CABBA/MECCA modelling tool kit.

It would have been good to see some impact of the updates carried out in terms of an evaluation of the chemical mechanistic updates against previous versions of MECCA/MOM as well as some evaluation against other chemical mechanisms, such as the more detailed benchmark MCM, over a range of atmospherically important chemical conditions. I realise that this is listed (and it is just a bullet pointed list) in the “Summary and outlook” section of the paper, but it is not clear if this work has been carried out, or is just a goal at the moment. In any case, some evaluation of the changes implemented in this version of CABBA/MECCA should be included in this paper before it is published in GMD.

More specific comments are given below:

- Perhaps mention “community model” in the title? (multi-purpose community atmospheric chemistry box model..)
- Introduction: A short descriptive definition of CABBA/MECCA and its history would be useful
- 2.1 Mainz Organic Mechanism (MOM) as the title
- Page 2, Line 14 – “explicit with a low degree of lumping” There for the scheme is not explicit!! More explanation needed here with respect to “lumping”.
- Page 2, Line 16 – The latest version of the MCM is v3.3.1, which is focused around a detailed update/evaluation to the MCM isoprene chemistry (Jenkin et al., Atmos. Chem. Phys., 15, 11433–11459, 2015). MIM2 is based on MCMv3.1. Therefore, it would be useful to see how the updated MECCA

model chemistry compares to MCMv3.3.1 in terms of isoprene chemistry under a range of representative conditions.

- Page 2, Line 25 - Given the last comment, what is the justification of not using the experimentally derived Crouse et al., (2012) 1,4H-shift kinetic data?
- Page 2, Line 31 – Updated aromatic chemistry. Has any evaluation of this updated chemistry been carried out against chamber data? How does it compare to other model aromatic atmospheric chemical mechanisms (the prediction of NO to NO<sub>2</sub> conversion and hence photochemical ozone formation, and chemical reactivity in various aromatics systems can vary significantly between different model chemistries.
- Figure 1. Please list species by category i.e. alkanes, alkenes, aromatics, oxygenates etc...
- Page 4. **2.1.1. VOC reactions with OH** – This section is severely lacking in detail with respect to the updates actually carried out and the impact of such updates. Specifically:
  - When were the IUPAC rate constants last updated? Referencing the IUPAC website datasheets as Atkinson et al., (2006) is somewhat out of date.
  - The updated substituent factors from the original SAR of Kwok and Atkinson need to be shown here (in a table) so that they can be compared/contrasted to other SAR approaches and so the methodology is transparent to the community.
  - “No rigorous evaluation of the SAR has been conducted and estimation uncertainty is expected to be in the same range as the MCM” I strongly recommend that an evaluation of the updated SAR is carried out and compared to the original and other SAR approaches used in other models/chemical mechanisms.
- Page 4. “2.1.2 RO<sub>2</sub> reaction with NO<sub>x</sub>” – Should be “with NO<sub>x</sub>” as you also look at RO<sub>2</sub> + NO<sub>3</sub>.
- Page 7. 2.1.4 RO<sub>2</sub> permutation reactions, Line 11 – “The rate expressions are not from the MCM, except...” The rate expressions “not from the MCM” need to be defined and put into a Table here.
- Page 7. 2.1.5 Photo-induced reactions – Line 15 (and through-out) define photolysis rates as “*j*-values”, i.e. *j*(NO<sub>2</sub>), and not “*J*-values” throughout.
- Define “HPALD and ”PACALD”
- Figure 3 appears before it is mentioned in the text
- Page 8. 2.2 Other chemical mechanisms – some discussions, even brief ones about differences in the chemical schemes, would be useful
- Again, some evidence of evaluation of the updated MECCA/MOM chemistry against older versions and other detailed chemical mechanisms (such as the MCM) is needed here.
- Page 11, Table 1. Needs much more explanation here. What is the colour coding in the table?
- Page 10, line 11 – “from a global atmospheric chemistry simulation based on...”, describe the scenarios used in this simulation
- Page 15, Line 13 – Figure 5 appears after the References?!
- Page 16. 4 MECCA in the MESSy modelling system – MESSy needs defining
- Page 20. Summary and outlook. Not actually a “summary” but a list of high level desirable goals. This should be re-written.