

Interactive comment on “The atmospheric chemistry box model CAABA/MECCA-3.0gmdd” by R. Sander et al.

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The authors have developed a new version of the atmospheric-chemistry box model CAABA/MECCA, integrating very different branches of code development into a single environment, in addition to an enhancement of already existing functionality. I believe the model represents an extremely valuable tool to study various different aspects of atmospheric chemistry.

The manuscript provides a detailed and much needed overview on the wide scope of the model, so that the user knows what is there and is informed about material that describes the different aspects in greater detail. In combination with the supplemental manual, the manuscript permits an efficient and sensible usage of CAABA/MECCA.

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The manuscript is, in general, well written and structured and I recommend it for publication in Geoscientific Model Development after minor revisions. Note that some of the points concern language issues and should be considered suggestions since I am not a native speaker of English.

Specific comments

1 The well written and extensive manual "caaba_mecca_manual.pdf" is much appreciated. Yet, it would be great if you included into Section 1 of the manuscript two or three sentences about the creation of a model setup via the xcaaba and xmecca shell scripts. You might also mention the namelist-guided control at run-time.

2 In my opinion, the headings "CAABA model description" and "MECCA model description" should each be followed by a short introduction to the respective Section. Subsection 2.5 appears somewhat out of place and you might consider moving it into the introduction to Section 2.

3 The summary is too short. It should, at least, sketch likely future developments of CAABA/MECCA.

4 p198.11 Remove "(GPL)"

5 p198.24 "as well as for" -> "and"

6 p198.23 Add a sentence defining the term "box model", maybe via the air parcel concept.

7 p198.26 Please define the term "global model". What about chemistry-transport models?

8 p199.10 "manual/ directory" -> "manual directory"?

9 p199.11-12 "should be consulted" -> "may be consulted"

10 p199.9 "(including rate coefficients and references)" -> ", including rate coefficients

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and references,"; a lot of text inside the brackets: would you please do similar replacements throughout the paper.

11 p199.17 "entrainment, emission, deposition" -> "exchange with air masses outside of the box"

12 p199.21-23 "Exchange with air masses ... SEMIDEP (simplified emission and deposition)" -> "The processes of entrainment, emission, detrainment, and deposition are calculated by the submodel Simplified EMIssion and DEPosition (SEMIDEP)". Please add a brief definition here of the processes entrainment, emission, detrainment, and deposition.

13 p199.footnote "bug fixes can" -> "bug fixes may"

14 p200.1 "there is no difference between entrainment from above and emissions from below" because transport inside an air parcel is not defined?

15 p200.equations1,2 Please provide an appropriate reference. Is the physics behind the boundary-layer height scaling associated with turbulent vertical diffusion?

16 p200.16 Would you please give a reference.

17 p200.22 "another" -> "a different"

18 p201.8 "allow" -> "permit"

19 p201.9 "The first" -> "One"

20 p201.10 "reaches" -> "reaches a"

21 p201.12-13 "to fix the physical ... to their measured values" -> "to use fix measured values for the physical"

22 p201.15 "yields insight how" -> "provides insight on"

23 p201.17 "for each data set measured at a given time" -> "per data set and time of measurement"

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24 p201.18 "over measured data sets" -> "over a number of measured data sets"

25 p201.22-23 Remove ", which"

26 p201.24 ", is now available officially" -> "and is now available"

27 p201.25-26 This sentence is hard to understand.

28 p202.2 Would you please give an example of a typical data source for the pre-calculated trajectories: ECMWF analyses, for instance?

29 p202.5 I guess the relevant quantities for the box calculations are pressure, temperature, relative humidity, radiation, and these depend on latitude and longitude? Would you please be more precise.

30 p202.7 "Exchange with surrounding air masses (mixing)" -> "Note that mixing with surrounding air masses"

31 p202.8 I assume the Lagrangian-style simulations do usually not stop at a steady state?

32 p202.paragraph1 In this paragraph, what is the benefit of TRAJECT over the steady-state mode? Is it more realistic?

33 p202.9 Remove "In addition to the ... model,"

34 p202.11 "can be" -> "may be"

35 p202.12-13 You are committing comma splicing. "global model" -> "global-model"; "the same chemical mechanism is chosen" -> "chemical mechanisms are identical"

36 p202.16 It is not evident from the manuscript why the contributions from mixing and chemistry can be separated. Would you please add a brief explanation in just a few words referring to Riede et al. (2009).

37 p202.20 "all levels of the atmosphere" -> "the whole atmosphere"

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- 38 p202.22 Remove "3-D"
- 39 p202.25 " ... stratospheric scenario": Is the user able to choose height and geographic location? "for 20 hPa" -> "for a height of 20 hPa"; does the initialization depend on latitude and season?
- 40 p203.1-2 Would you please specify the model in Jöckel et al. (2006).
- 41 p203.14 "size bins" -> "bins of aerosol radius, hereafter referred to as size bins"
- 42 p203.23 "loss" -> "loss rate" ?
- 43 p203.26 "can" -> "may"; remove "primary"
- 44 p204.1-2 "If there ... consist of" -> "In case there is difference in the ?number? of ... , it is compensated by ... "
- 45 p204.6-7 "because they ... gas phase." -> "due to the interaction with the gas phase."; "has been used recently" -> "has recently been used"
- 46 p204.8-9 "to ship-borne measurements of marine aerosol" -> "of ship-borne marine-aerosol measurements"; what is a "6-stage cascade impactor"? You might consider either a short explanation or remove the phrase.
- 47 p204.11-12 What factors contribute to the uncertainty? "how the model results depend on" -> "how sensitively the model reacts to"
- 48 p204.15 Do you vary a single parameter for every simulation, or several parameters at the same time?
- 49 p204.17-18 "kinetic" -> "rate-coefficient"? "As another example" -> "To give a further example"
- 50 p204.18 "O3 changes" -> "O3 mixing ratios change"; please do similar replacements throughout the paper, also in the caption to Figure 4.
- 51 p204.24 "random" -> "pseudo-random"; likewise throughout the paper

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- 52 p204.24 "Dlogk" -> "The uncertainty Dlogk"
- 53 p204.25 Remove "it is"
- 54 p204.26 "http" -> "see http"
- 55 p205.1-2 "to generate ... numbers" -> "to transform uniformly into normally distributed pseudo-random numbers."
- 56 p205.5 Remove "can be used" and "potential"
- 57 p205.7 "numbers" -> "number sequences"
- 58 p205.7-9 Replace sentence by "The Mersenne-Twister algorithm should be used in case identical sequences are required with different compilers."
- 59 p205.11 "The main ... on" -> "The mechanism development focused on"
- 60 p205.13 I don't understand the notation Hg(0).
- 61 p205.14 "global significance": significance with respect to the global distribution of Hg mixing ratios?
- 62 p206.8 Remove "rather"
- 63 p206.27-28 Replace sentence by "It is thus suitable for assessments of carbon-isotopic trace-gas composition and CO production from biogenic sources."
- 64 p207.18-20 Begin the sentence with "Considering the complex chemistry ... "
- 65 p207.22 "Isotope chemistry" -> "Isotope-chemistry modeling"; "accounting for the" -> "consideration of"
- 66 p207.25 "one" -> "a single"
- 76 p207.27. "reactions" -> "reaction"
- 68 p207.6 "H, S, N" looks odd; maybe use "hydrogen, ..." instead?

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69 p207.heading3.7 "Further recent changes" -> "Further changes"

70 p208.12 "can be found" -> "is available"

71 p208.23 Change clause into: "It provides a greater number of different numerical integrators."

72 p209.1-2 "allows output of the" -> "allows the output of"; "of selected" -> "associated with the selected"; "Alternatively," -> "Alternatively, the"

73 Figure3 "A illustrative comparison" -> "Illustration"; do you know the conditions encountered at the boxes? Maybe add something like "trajectories (black arrows), flight path (red arrows)".

74 Figure4 A short description of the model setup would be helpful.

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