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## ***Interactive comment on “The atmospheric chemistry box model CAABA/MECCA-3.0gmdd”***

### **by R. Sander et al.**

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We would like to thank Rudolf Deckert for his very useful comments. Replies to his suggestions are embedded below.

1 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.

As suggested, we have added some text. However, we think that it fits better into the CAABA model description section than into the introduction.

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.

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Changed as suggested.

Subsection 2.5 appears somewhat out of place and you might consider moving it into the introduction to Section 2.

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Changed as suggested.

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

We have several ideas for code development in the future. As requested, we now mention some ideas in the summary.

4 p198.11 Remove "(GPL)"

Changed as suggested.

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

Changed as suggested.

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?

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The introduction now contains a short definition of the terms box model and global model.

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

Changed as suggested.

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

Changed as suggested.

10 p199.9 "(including rate coefficients and references)" -> ", including rate coefficients and references"; a lot of text inside the brackets: would you please do similar replacements throughout the paper.

Changed here and at several other places.

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

Changed as suggested.

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

This footnote was specific to the discussion paper and has been removed completely.

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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.

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

The sentence was changed as suggested and it is now mentioned that, for a box model, these processes are simply fluxes into or out of the box.

15 p200equations1,2 Please provide an appropriate reference. Is the physics behind the boundary-layer height scaling associated with turbulent vertical diffusion?

The references were added as requested. In the box model, there is no physics behind the boundary-layer height. It is simply an input parameter for the model.

16 p200.16 Would you please give a reference.

We refer to our previous model version by Sander et al. (2005), which has now been added as a reference here.

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

Changed as suggested.

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

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Changed as suggested.

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

Changed as suggested.

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

Changed as suggested.

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

We find the formulation "to use fix measured values" difficult to understand and prefer to keep the sentence unchanged.

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

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Changed as suggested.

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

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Changed as suggested.

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

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Changed as suggested.

25 p201.22-23 Remove ", which"

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

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Changed as suggested.

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

An additional explanation has been added.

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?

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

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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).

The section about Lagrangian trajectories has been rewritten to consider these comments.

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

We would like to keep this part since the basic functionality as a trajectory-box model is independent of its application as an analysis tool for global-models results within the MESSy framework.

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

Changed as suggested.

38 p202.22 Remove "3-D"

We prefer not to remove "3-D" because it is not redundant. Not all global models are 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?

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Typical values for initializing the chemistry at 10 or 20 hPa are available. Further values for other pressure levels, latitudes or seasons can be added if needed. This information has been added to the text. Since 20 hPa is a pressure level and not a height, we prefer not to rephrase the sentence to “a height of 20 hPa”.

40 p203.1-2 Would you please specify the model in Jöckel et al. (2006).

Changed as suggested.

41 p203.14 "size bins" -> "bins of aerosol radius, hereafter referred to as size bins"

Changed as suggested.

42 p203.23 "loss" -> "loss rate" ?

Changed as suggested.

43 p203.26 "can" -> "may"; remove "primary"

Changed as suggested.

44 p204.1-2 "If there ... consist of" -> "In case there is difference in the ?number? of ... , it is compensated by ... "

For clarification, we changed “amount” to “concentrations”.

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45 p204.6-7 "because they ... gas phase." -> "due to the interaction with the gas phase."; "has been used recently" -> "has recently been used"

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Changed as suggested.

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.

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Changed as suggested.

47 p204.11-12 What factors contribute to the uncertainty?

We think that a description of the uncertainties associated with laboratory measurements are not within the scope of this model paper.

"how the model results depend on" -> "how sensitively the model reacts to"

Changed as suggested.

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48 p204.15 Do you vary a single parameter for every simulation, or several parameters at the same time?

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All parameters are varied at the same time, this is now explained better.

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49 p204.17-18 "kinetic" -> "rate-coefficient"? "As another example" -> "To give a further example"

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Changed as suggested.

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50 p204.18 "O3 changes" -> "O3 mixing ratios change"; please do similar replacements throughout the paper, also in the caption to Figure 4.

Changed as suggested.

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51 p204.24 "random" -> "pseudo-random"; likewise throughout the paper

Changed as suggested.

52 p204.24 "Dlogk" -> "The uncertainty Dlogk"

Obsolete, since details about obtaining  $\Delta \log k$  have been moved into the supplement.

53 p204.25 Remove "it is"

Changed as suggested.

54 p204.26 "http" -> "see http"

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Changed as suggested.

55 p205.1-2 "to generate ... numbers" -> "to transform uniformly into normally distributed pseudo-random numbers."

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Changed as suggested.

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56 p205.5 Remove "can be used" and "potential"

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57 p205.7 "numbers" -> "number sequences"

Changed as suggested.

58 p205.7-9 Replace sentence by "The Mersenne-Twister algorithm should be used in case identical sequences are required with different compilers."

Changed as suggested.

59 p205.11 "The main ... on" -> "The mechanism development focused on"

Changed as suggested.

60 p205.13 I don't understand the notation Hg(0).

In chemistry, a number in brackets after the element symbol is used to describe the oxidation state. Thus, Hg(0) refers to elemental mercury.

61 p205.14 "global significance": significance with respect to the global distribution of Hg mixing ratios?

Changed as suggested.

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62 p206.8 Remove "rather"

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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."

Changed as suggested.

64 p207.18-20 Begin the sentence with "Considering the complex chemistry ... "

Changed as suggested.

65 p207.22 "Isotope chemistry" -> "Isotope-chemistry modeling"; "accounting for the" -> "consideration of"

Changed as suggested.

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66 p207.25 "one" -> "a single"

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Changed as suggested.

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76 p207.27. "reactions" -> "reaction"

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Changed as suggested.



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"

Changed as suggested.

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

Changed as suggested.

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

Changed as suggested.

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

Changed as suggested.

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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)".

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Changed as suggested.

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

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We have added that the model run was made using tropospheric conditions and gas-phase chemistry without any non-methane hydrocarbons.

Interactive comment on Geosci. Model Dev. Discuss., 4, 197, 2011.

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