gmd-2024-166 – Reply to referees

We thank the referees for their constructive comments. In the course of the open discussion we have become aware of a minor bug in the diagnostics of KPP substeps for the aqueous-phase chemistry in aerosols as implemented in AERCHEM. However, only the absolute numbers change and the relative change is almost identical. We have changed Table C1 with the correct values.
In the following, we have listed the comments in normal font color and style, followed by our replies in blue and modifications to the text in red.

Referee #2

This is a nice paper examining how step size control/optimization impacts computational efficiency and accuracy when simulating atmospheric (multiphase) chemistry in box and 3D global chemical transport modeling. It is relatively clear and well-written and presents novel results that will be of significant value to atmospheric chemistry modeling community, particularly for operational 3D modeling where efficient yet accurate approaches are required. It is well-suited for GMD. I recommend publication with the consideration of minor edits/questions.

We thank Referee #2 for the very encouraging review. Here below we address the questions.

1) Line 67. From "represents the currently used controller used in our applications that we investigate" to "represents the controller we investigate. . . "

We will change this accordingly.

2) Line 91. From "robuster" to "more robust"

We will change this accordingly.

3) Table 1 caption. Change "over" to "of"

We will change this accordingly.

4) Lines 127-132. Are these three scenarios specified only by changing input parameters or are there changes to the mechanism treated? (You might want to mention this here and define the changes that are made to represent the different scenarios somewhere.)

Yes, the three scenarios are among the available scenarios of the CAABA/MECCA model. They are specified by setting different input parameters and emissions. We will mention this more explicitly and add references that include the initial concentrations and emissions.

5) Line 145. Remove the word "binary"?

We will change this accordingly.

6) Line 153. Should "GMXE" be changed to "GMXe"?

We will change this accordingly.

7) Lines 186-187. This is unclear to me. Output is written every 23rd hour? Or every day at hour 23? How does this lead to output for every hour of the day? Do you just mean that there are outputs for each hour (0-23) as you cycle through the days of the year (writing every 23rd hour) but not outputs for every hour of each day?

It is every 23rd hour so that for each subsequent simulated day the output is at a local time one hour earlier. Therefore, after 24 days we would have output for each local hour (0-23) of the day. This allows to sample the model state in fairly all the chemical regimes. We will rephrase it to make it more clear.

8) Line 233. Typo – change "suite" to "suit"

We will change this accordingly.

9) Line 262. Remove "for qmax" (redundant)

We will change this accordingly.

10) Line 272. From "decreasing" to "decrease".

We will change this accordingly.

11) Line 279. From "good" to "well".

We will change this accordingly.

12) Line 281. From "tough" to "though".

We will change this accordingly.

13) Line 301. From "scenario, respectively." to "scenarios."

We will change this accordingly.

14) Section 4.1 and elsewhere (e.g., line 315): it might be better to say "fewer" function evaluations than "less".

We will change this accordingly.

15) Also, any thoughts on why the qmax changes had more influence in the global simulations wrt MECCA compared to SCAV and the box modeling where it was not very impactful?

The most likely reason for this is, that the MECCA chemical mechanism in the global simulations does not cover the aqueous phase chemistry, making it less stiff. Especially in the stratosphere during nighttime the solution for some model time steps only requires very few sub steps. However, with the default qmax value of 6 the step size can't increase fast enough from the small step size that is required at the beginning of the model time step. Because of this the solver will calculate much more sub steps than the ODE system would need. So the default qmax value kind of implicitly introduced a lower limit of sub steps that will be calculated, which is unnecessarily high for the MECCA/EMAC case.

16) Line 326. Change “over” to “of”.

We will change this accordingly.

17) Table 3 caption: Change from “qmax and [safety factor] for MECCA and SCAV” to “qmax and [safety factor] for MECCA, [safety factor] for SCAV,”. Change “brackets” to “parentheses”.

We will change this accordingly.

18) Line 361. Remove comma.

We will change this accordingly.

19) Line 365. From “an precision” to “a precision”

We will change this accordingly.

20) Line 377. Change “areas” to “area”

We will change this accordingly.

21) Line 380. Remove “proceeded rather consistent and”?

We will change this accordingly.

22) Line 390. What is this reference?

Thank you for pointing out a mistake here. We will change the reference to be displayed correctly.

23) Would it be worthwhile to look at the relative differences for an aerosol species that has important chemistry in cloud and aerosol water (e.g., sulfate)?

We think that this is a good suggestion. We added plots with relative differences of SO_4^{2-}, NO_3^-, NH_4^+ and Cl^- as supplementary material and at the end of this reply. For these species the relative differences were within an acceptable range either. Accordingly, we have added the following text to line 395:

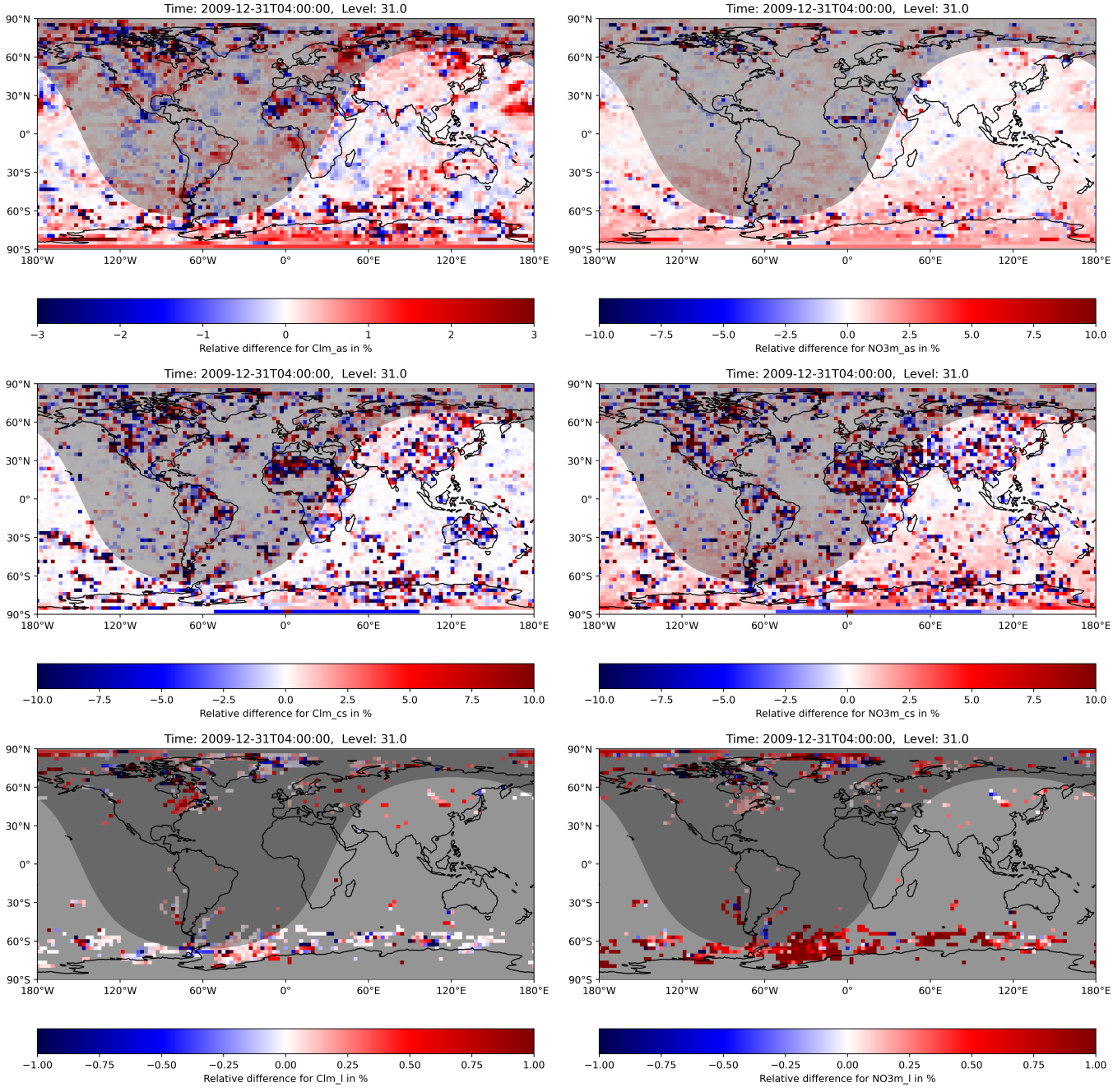
For completeness, we added the relative differences for NO_3^- and Cl^- (Figure S1) and for SO_4^{2-} and NH_4^+ (Figure S2) in their respective aqueous and aerosol-phases as supplementary material.

24) Line 423: Change “worth” to “worthwhile”

We will change this accordingly.

25) Line 448. Change “. . . to the Eq. 6, we only have two” to “. . . to Eq. 6 with only two”

We will change this accordingly.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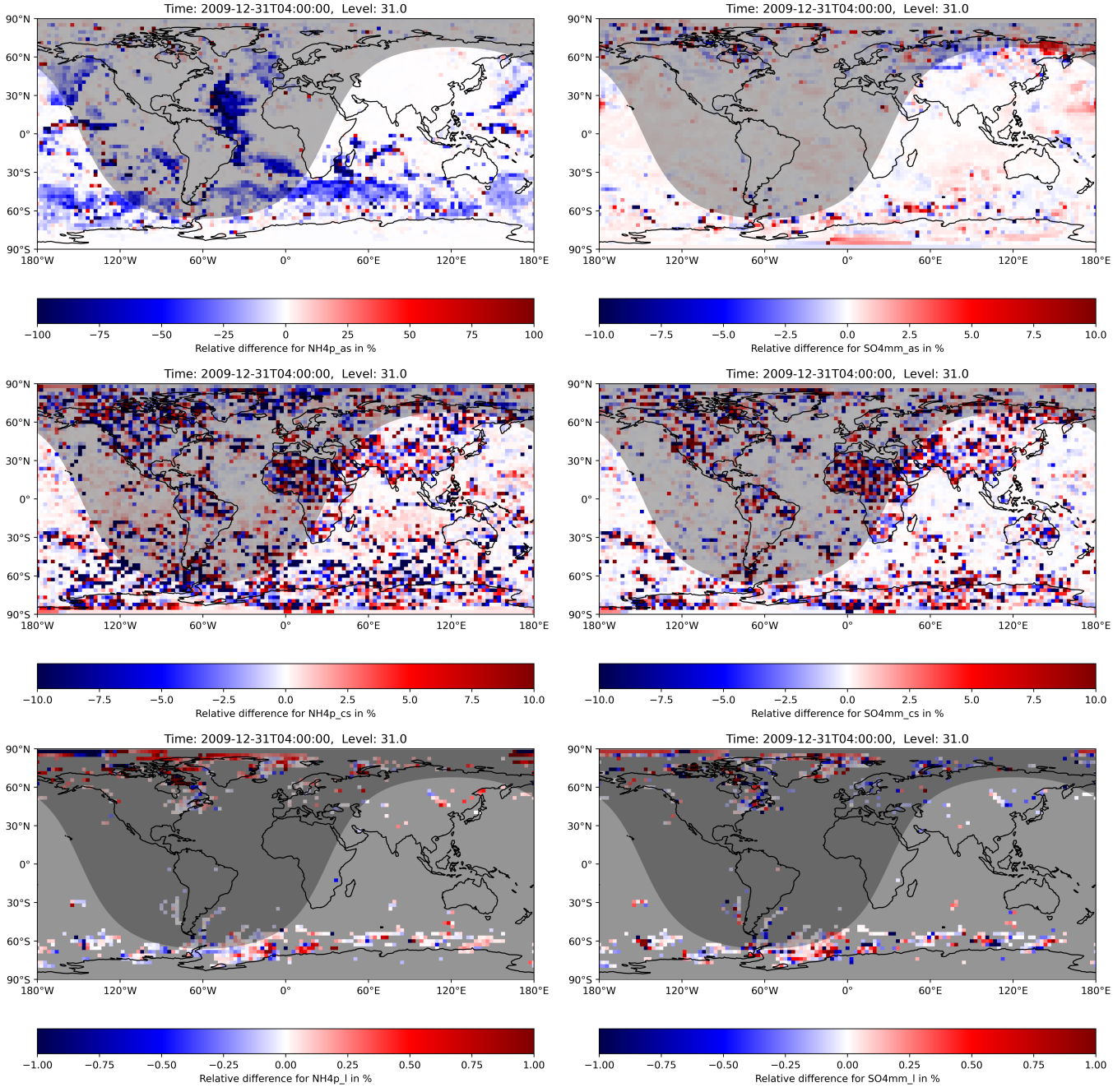
Relative difference for NO3m_l in %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Relative difference for NH4p_as in %
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Relative difference for NH4p_cs in %
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Relative difference for NH4p_l in %
Time: 2009-12-31T04:00:00, Level: 31.0
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Relative difference for SO4mm_l in %

References