Geosci. Model Dev. Discuss.,
https://doi.org/10.5194/gmd-2020-110-RC1, 2020

Geoscientific Model Development Discussions
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Interactive comment on "Description and evaluation of a detailed gas-phase chemistry scheme in the TM5-MP global chemistry transport model (r112)" *by* Stelios Myriokefalitakis et al.

Anonymous Referee #1

Received and published: 27 May 2020

This work reports on the implementation of an extended VOC chemical mechanism and the Rosenbrock solver into the global TM5 model. In addition, the model is evaluated with respect to the performance of the original, the new integrator, and the new VOC mechanism. Observational comparisons are used to quantify the performance of the new model advances.

Even though both concepts, the use of the Rosenbrock solver in global models and the implemented VOC chemistry, are not novel, the advancement for the TM5 community is still considerable. However, I have substantial concerns regarding the model

description, the model analysis, and the presentation of the complete manuscript in general.

As such, I believe that major revisions are necessary before this manuscript is ready for publication in GMD. In the following, I present first the major concerns, followed by specific comments and technical corrections.

General comments:

I have multiple concerns on how the model is described within this manuscript. Very little general information on the TM5 model is provided, except for a long list of citations. For a non TM5 community member it is impossible to understand the key features of this model without opening another publication. A general description of the model needs to be provided, especially since many discrepancies in the model comparison are attributed to transport processes. A summary on how transport processes are simulated needs to be added. An additional evaluation of these transport processes would be useful to justify the later claims. Additionally, some information that should be included in the model description can be found in later sections (e.g. how the tropopause altitude is calculated between the different simulations). The manuscript should be harmonised such that all these information are included in the model description.

Within this study, two different chemical mechanisms are used but the manuscript only includes information on the newly developed one. A short description on the "standard" TM5 mechanism should be included and a list of all reactions of this mechanism needs to be added to the supplemental material. A box model comparison of all mechanisms (i.e. MOGUNTIA, CB05 and MCM) would be useful to understand the mechanistic differences. Within the text it becomes evident that different emission data sets are used for the different mechanisms. However, this information is not at all included in Section 2.4. The emissions for the standard mechanism need to be provided (e.g. table in supplemental material).

Scientifically, many claims on what causes the differences between the model and the observations are not supported by the provided data and not enough evidence is given. In one particular case, too low upward transport is given as a reason and one page afterwards it is claimed that the model simulates a too high transport in the same region. The manuscript therefore needs to be checked if the claims are supported by the results. If so, more justification must be provided (e.g. presenting differences in O_3 precursors). Otherwise these statements should be removed.

All in all, the model tends to underestimate VOCs, which is mainly attributed to too low emission sources. Higher emission strengths of VOCs will lead to higher VOC concentrations in low-NOx regime, influencing the O_3 production. I therefore strongly suggest to perform a sensitivity simulation with up-scaled emission sources to investigate the impact on O_3 and HO_x.

Another major concern I have is the overuse of citations when referring to earlier work. A good example is page 4 line 17-20: This sentence has 12 citations but only 18 words with providing no important information about the model at all. It feels as if every paper that used the model is cited here (without evidence why this is necessary), which should not be the goal of the model description. It should be sufficient to cite e.g. Huijnen et al., 2010 since they focus on the chemical modelling in TM5. The same holds when referring to earlier studies using parts of the mechanism (e.g. page 6 line 6-7, page 6 line 32, page 7 line 3-4), especially if they are not further used in the manuscript. It would be scientifically more profound to only cite publications, in

which the approach was novel or were it was used first and not every publication using this part of the mechanism or model development. I therefore strongly advise you to recheck every citation in the manuscript and limit citations to a minimum.

Last but not least, when reading the manuscript it does not feel like a coherent story and each section feels like an isolated section. Additionally, the manuscript suffers from grammatical mistakes. I therefore suggest sweeping through the document focusing on simpler sentence structures.

Specific comments:

Page 1:
Line 31-33: Not much information is given about other global models in your manuscript. Therefore, you should only focus this statement on TM5.

Page 4:
Line 28-29: What influence does this approach have on the stratospheric-tropospheric exchange in your budget analysis?

Page 5:
Line 4-5: When using 150 ppb as definition, the tropopause altitude will differ when using different chemical mechanisms or integrators. Do you use the same tropopause altitude for each simulation? And if so, on which simulation is this definition based? Is the tropopause altitude calculated for each time step or is it based on mean data? What impact do you expect from this?
Line 7: The only O_3 chemical aqueous-phase sink considered here is SO_2. However, the major aqueous-phase sink of O_3 is the reaction with O_2^- (Liang and Jacob, 1997).

By not taking this sink into account, what impact do you expect this has on the O_3 budget and the O_3 burden in your analysis?

Page 7:
Line 13-15: Due to the citation style used, it is not at all obvious in which publication each of the advances have been published.
Line 26: How are meteorological conditions simulated in TM5? This needs to be discussed in the general description of the model (Section 2.1).

Page 8:
Line 23-26: This information is useful to understand why KPP was implemented into TM5. I would suggest you mention this first (i.e. page 8 line 8 and in the introduction).

Page 10:
Line 12: What complexity has the chemical mechanism used for mCB05? Provide more information about this mechanism.

Page 11:
Line 1-15: How is this model performance analysis performed (e.g. which software)? What are the expected limitations?
Line 2-4: This information should be included in Section 2.5.
Line 8-9: The transport of tracers seems to be important for the model performance. How is it decided which tracer is transported and which not? This should be discussed in the model/mechanism description.

Page 12:
Line 7-9: This is not clear. Why is the chemical destruction higher due to changes in

the O_3 precursors?
Line 8-9: How do the changes in the O_3 precursors look like? This is a nice example were a statement is given without providing any results or argument why this must be the case (see general comments).
Line 12: Why is it necessary to used NO_y mass fixing when using EBI? This needs to be discussed in the model description since this is a major difference between EBI and KPP!
Line 19: This is unclear. By referring to table 3 it implies that different emission datasets are used for the different simulations. If so, why is that the case? This needs to be elaborated in Section 2.4.

Page 13:
Line 4: With the 150 ppb definition your simulation are already up to 15% higher. How does your model compare to Lamarque et al. (2012) when using 100 ppb as tropopause definition? It would be best to provide both budgets (i.e. in Table 4) for the 100 and 150 ppb definition to allow a fair comparison.
Line 13: It is not at all clear in Section 2.4 that different emissions are used. What is the impact of using different emissions?
Line 30-31: This is a good argument for the model description to justify why this approach is used.

Page 14:
Line 4: The contribution of the “other reactions” changes from about 200 to 120 Tg/yr. What causes these changes and what is included in this category?
Line 9-10: This should be mentioned in the model description.
Line 12: Which tropopause definition did van Noije et al. (2014) use?
Line 27: The difference is about 15%, so using “somewhat shorter” is a slight underestimation.

Line 34: What lifetime do you get when using 100 ppb as tropopause definition?

Page 15:
Line 9: To what else can these differences be attributed to?

Page 17:
Line 18-19: This is a bit confusing. The dataset used to compare 2006 is published in 2000? What are the limitations of this comparison when using different years?

Page 18:
Line 21-22: Due to the lack of specific details on mCB05 in the manuscript, it is impossible to identify why this must be the case. More details are necessary here.
Line 24: Provide more details on how NOx reservoir species differ in their concentration and spatial distribution between both mechanisms.

Page 19:
Line 2-3: How well does your model compare when using 7.9Tg-N/yr?
Line 14-17: Provide evidence why this is the case.

Page 20:
Line 3: What about comparing your model simulations to satellite observations of O_3 (e.g. OMI)?
Line 18-20: The surface ozone bias is lowest for mCB05(KPP) but at the same time the ozone burden is higher than for MOGUNTIA. What causes this difference? Are there significant differences in free tropospheric ozone?

Page 21:
Line 10-11: This conclusion is not obvious based on the results you provided. Further analysis is needed here. How well are transport processes modelled in TM5?
Line 15-18: Are these speculations or do you have evidence that this must be the case? If so provide further details.
Line 32: This statement is unclear. The current sentence structure implies that the emissions in the SH are lower when using KPP.

Page 22:
Line 21-23: Earlier (i.e. page 21, line 10-11) you state that the convective uplift is too low but now you state that it is too strong. Which is correct? The presented data do not support either. More evidence is needed. I strongly suggest you to perform an elaborated analysis of the performance of TM5 with respect to transport processes, to justify these claims.
Line 24-25: Have you analysed biomass burning hotspots to support this claim?

Page 23:
Line 2: What causes the opposite annual cycle?
Line 9: Your model underestimates propane but you use a lower emission than other studies. How does your model compare when you use higher emissions?

Page 24:
Line 1-2: Could this underestimation be related to underestimated transport processes (see Page 21 & 22)?
Line 20: What needs to be done to account for the “secondary production from VOC oxidations”?

Page 25:
Line 30-33: Can you provide some suggestions on how to improve these uncertainties?

Page 53:
Table 4: What about O_3 scavenging?

Technical corrections:

Page 2, line 4-20: A graphical illustration of the NO_x-VOC-O_3 relation would be helpful here.
Page 4, line 22 & Page 14, line 1-2 & Page 18, line 11-13: Check gramma and wording.
Page 5, line 3: The statement that this study focuses on the troposphere is stated multiple times. Do not use double statements, to improve the reading flow.
Page 6, line 1: This should be Section 2.2.
Page 9, line 10-14: Listing all species greatly disturbs the reading flow. I would remove this listing and just refer to Table 3 instead.
Page 10, line 12-28: A table summarizing all simulations performed could be useful.
Page 12, line 22-26: This is a rather complicated sentence. Consider using simpler language (i.e. multiple short sentences).
Page 14, line 26: The word “arrive” should not be used here.
Page 17, line 2-19: Presenting the different observations and possible comparisons in a table would be more efficient.
Page 17, line 25: In order to improve the reading flow, it would be best to first compare each tracer discussed in Section 4 (in the same order).
Page 20, line 25: Is the reference to the introduction correct?
Page 20, line 27: Please be more specific and refer to Section 2.1.
Page 41-51: Most of the information presented in Tables 1, 2 and even 3 are well

documented elsewhere. Thus, I strongly recommend you to move these tables to the supplemental material.
Supplement, page 3: Table S3 (including caption) cannot be read completely.

References:
Liang, J. and Jacob, D. J.: Effect of aqueous phase cloud chemistry on tropospheric ozone, Journal of Geophysical Research: Atmospheres, 102, 5993–6001, https://doi.org/10.1029/96JD02957, 1997.

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