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Interactive comment on "Methane chemistry in a nutshell – The new submodels CH4 (v1.0) and TRSYNC (v1.0) in MESSy (v2.54.0)" *by* Franziska Winterstein and Patrick Jöckel

Anonymous Referee #1

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Methane chemistry in a nutshell – The new submodels CH4 (v1.0) and TRSYNC (v1.0) in MESSy (v2.54.0) , Winterstein and Joeckel, GMD-2020-137.

This GMD paper presents a description of a submodel for use in the Modular Earth Submodel System (MESSy) to describe the role of methane and its isotopologues in a reduced complexity treatment. The idea is that the CH4 submodel can be used in a variety of different configurations, some of which may choose to exclude full chemistry for reasons of computational cost, and yet use of the submodel will retain a more detailed treatment of methane and its impact than simple climatologies. The oxidant fields supplied can be from existing simulations, previously run models, or within the

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simulation from more explicit chemical submodels. The paper describes the underpinning methods in the submodel, and examples where the submodels is applied to emissions inversions, simulation of isotopologues of methane and production of water isotopologues from methane oxidation.

Presentationally, the manuscript is well written and interesting. However, the model set up is mostly explained via schematics that are novel in form but regrettably not as clear as a flow chart or diagram would be. I don't feel that the diagrams, particularly Figure 1 and S1, are sufficiently clear enough to represent the mechanism or equations in use, and these should be included instead, or references supplied.

The paper describes a submodel already somewhat extensively described by Eichinger et al, 2015a, reference in this paper, and this does potentially diminish its novelty. I think it would be important to add a clear section on any differences between the implementation described here and that already in Eichinger et al.

Given that the abstract makes plain that a key area of interest is simulating stratospheric water vapor production, the lack of an assessment of the skill of the submodel in this latter regard is noticeable. I feel the paper would be strengthened, and the assessment of the submodel for SWV simulations improved, if a further section were added on this point. I appreciate that this is difficult given the underpinning model biases, but I would suggest, in particular, that the use of instantaneous production of 2 water molecules per CH4 oxidised might be assessed further, and it may also be interesting to ask, What is the impact of the use of the CH4 submodel on radiative forcing from all relevant species, that is H2O, CH4 and O3 vs a model in which the effect of CH4 on SWV was excluded?

Conceptually this paper has a sound idea to reduce the difficulties in simulation of methane's impact on radiative forcing to a simpler submodel, and the implementation appears to be well thought through.

I think the paper would be improved by the addition of more detail on the impact of the

choices made, particularly considering the processes or feedbacks that it was necessary to omit or treat at a reduced level of detail in the submodel and how these choices impact model skill.

Assessment of the correctness of the implementation of the atmospheric feedbacks is important here, and it is unfortunate that the concept of feedback is used somewhat broadly, which slightly obstructs the reader's own assessment of what the feedbacks are between or how they arise and whether they are implemented correctly. A key feedback is that of CH4 on OH, yet the specific examples do not mention OH, or the generation of species which could be the sink for OH, such as CO. Mention is made of HO2, however.

Similarly, the use of the phrase 'predefined fields' could be made more explicit to indicate the coupling

L7: – is the oxidation always 'offline', that is the loss of OH is not returned to the chemical solver as a feedback?

L131: the model can be coupled to, but what is the nature of the coupling? One-way (submodel receives oxidant fields) or two-way (submodel returns depleted OH, Cl fields to MECCA)?

L 138: 'secondary feedback': implies that there is feedback, but of which species? Figure 1: what do the green and black lines signify? What is the meaning of the differently shaded arrows? What is the meaning of yellow and red species?

Figure 1: caption has what I believe should be in the text 'predefined fields without feedback' – but what about the effect of HO2 on OH?

L145: Would it be possible to add what the effect of this approximation is? Does H2O feedback on stratospheric ozone?

The level of detail is mostly good: section 1 focuses on the state of our knowledge of methane chemistry and emissions, as well as the underpinning reasons and methods

for simulation of isotopologues. Section 2 descrbes the MESSy model and associate submodels. Section 3 presents the submodel in schematic form and a lengthy treatment of the treatment of the ageing of methane, which looks like new material and an important step forward from the Eichinger paper, section 4 is also new compared to Eichinger, I believe, and describes the treatment of the water isotopologues. Section 5 presents three brief examples of the application of the submodel.

Overall this is a useful description of the CH4 submodel and the improvements made since the earlier publication. I consider that t is suitable for publication having addressed these general comments and specific suggestions below.

Detailed comments

L13: what does 'similar to' mean here more precisely? What do you mean by 'feed back' to the isotopological hydrological – do you mean 'is passed back'?

L43: remove comma between both, natural

L46: what do you mean by 'not sufficiently accurate' here? Do you mean the lifetime is too short?

L56: reference required?

L60: Earth's surface

L74: rate constant not rate, given what comes after in the text

L80: k is usually reserved for rate constant but this is of course correct

L114: insert 'to' so as will read 'submodel to represent'

L186: modify 'is not conform with'

L193: modify 'to be conform with'

L200: drop comma between 'choose, whether'

L220: would make more sense as a list: 1) the CH4 submodel, 2) MECCA_TAG and 3) H2O. . .

L221-222: drop ‘are treating’

L231: ‘doubles’ is not very clear: do you mean ‘duplicates’?

L303: replace ‘most and largest’ with ‘most importantly’?

L306: sentence is rather inelegant.

L308-317: values are required for quantitative comparison.

Code availability I am not an expert on Copernicus policies, but it would appear that a DOI for the code will ultimately be required.

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