Climate of the Past Discussions

Clim. Past Discuss., referee comment RC2
https://doi.org/10.5194/cp-2021-150-RC2, 2022

Comment on cp-2021-150

Colin Goldblatt (Referee)

Referee comment on "Dynamics of the Great Oxidation Event from a 3D photochemical–climate model" by Adam Yassin Jaziri et al., Clim. Past Discuss., https://doi.org/10.5194/cp-2021-150-RC2, 2022

This manuscript concerns the Great Oxidation of Earth's atmosphere, with one of the first treatments of the chemistry in a GCM, and discusses possible links to the Palaeoproterozoic glaciations. The manuscript uses a mix of 3-D and 1-D photochemical modelling, and additionally uses a simple box model to explore some of the implications of the photochemical modeling results. These two methods are quite different, so I have separated my review into two parts to address them both.

The manuscript is on a very interesting topic, and uses an appropriate set of methods. I recommend that it will be suitable for Climate of the Past after suitable revision.

Photochemical modelling

Summary comments: I'm really happy to see some 3-D work on the oxygen photochemistry, but I think the presentation of the 3-D results is quite lacking, so the (no-doubt) interesting results from the modelling work are not made available to the reader! Also, much of the work presented and used in the manuscript is actually from a 1-D model, and clearer distinction of this needs to be made. Statements about code availability, sufficient explanation of the methods to realistically enable reproduction, and an archive of model output are needed.

There is not sufficient information in the methods to allow the work to be repeated. Via online repositories of code and/or machine-readable supplementary information, it is now possible to make modelling work genuinely reproducible. This should be done. If for some reason this cannot be done, an exceptional justification is necessary. There is no statement about the availability of the codes used in the manuscript, which is necessary (are the codes open source? If not, how can they be acquired?). Complete sets of inputs need to be provided (what are the actual boundary conditions for each model run – e.g.

what fluxes of which reductants are used?). A machine readable version of Appendix A should be included. Some details are vague (e.g. line 108 speaks of an eddy diffusion coefficient, whereas typically a vertical profile of these are used) – all details need to be clear.

There no archive of model outputs, which should be important, especially for the GCM runs which are very costly to produce. I would recommend, in the strongest terms, that authors make their data (model output) available following FAIR principles (https://www.go-fair.org/fair-principles/). Providing this to other researchers will add significant value to the manuscript.

The photochemical models use fixed mixing ratio boundary conditions at the surface. An excellent recent paper by Gregory et al. (2021) compares fixed mixing ratio and fixed flux boundary conditions, and concludes that fixed flux boundary conditions are preferable. This should be discussed, and the approach used here justified in that context, including discussion of any bias that fixed mixing ratio boundary conditions might introduce.

You note that the ozone column is large in 1-D (line 150). Is this a genuine difference between 1-D and 3-D approaches, or is your zenith angle simply poorly tuned in the 1-D model, given knowledge of the 3-D results?

The justification for using methane fluxes as a proxy for oxygen fluxes (line 163-4) is not clearly justified. Use of molecular oxygen to oxidize CO (which I suspect you include as a boundary condition) would plainly be an oxygen loss. You need to be clearer about why this is excluded.

Overall, I found the presentation of the results from the 3-D modelling a disappointment. There is only one figure which shows anything other than global means (Fig 5, which shows vertically resolved zonal means). Surely there are actually some interesting results in 3-D?! Conversely, if there really are not, then it would be a great service to the community to robustly make the case that 3-D models are quite unnecessary for this problem, so that no-one else need bother!

To be clear here: I strongly recommend more detailed presentation of the results from the GCM. For example, the questions that I would start with are: What is the model climatology of ozone and water vapour above the tropopause, and how does this compare to climatology? What is the model Brewer-Dobson circulation, and how does this compare to climatology? Note that this may well affect the ozone distribution, and how the rates differ from 1-D. How do these change with model temperature? Is there any feedback between changed ozone levels and the climate?

I am a little surprised by how cold the stratosphere gets. Does your radiation scheme

include near-IR absorption by methane, which has been shown to cause significant warming in 1-D models (Byrne & Goldblatt, 2015)? Also, note that at line 205 you refer to 220 and 280K, whereas Figure 12 shows results for 260 and 280K.

In appendix B, dominant photochemical pathways are presented. However, there is no discussion of the methods by which they were found, which is necessary. As with all the methods, this discussion should be sufficient for these to be reproducible, including reference to the codes used. There is no substantial discussion of these in the text of the manuscript, which would be important to contextualize them.

There has been prior work that has used 3-D models to examine atmospheric oxygen photochemistry, which should be referenced (e.g. Cooke, 2022).

Minor comments

Line 103: Orbital period in days is confusing if day length is changed.

Eq 6: Use a symbol in place of 'dens'

Line 139: define vmr

Line 140: "These results are consistent with the previous study by Zahnle": if you are making this point, you must show this to the reader. Include results from Zahnle in your graph (scrape from his graphs if necessary).

Figure 4: is too small to read – make bigger, for readers with older eyes! Also, the x-axis is truncated before -10^{-16}, which appears to mean that much of the structure is lost for low oxygen runs; show these lower magnitudes too.

Line 188: What do you mean to imply with "the tropospheric temperature profile follows a moist/dry adiabat"? That it is prescribed as such?! Presumably the GCM has more physics than that? Or are you talking about the 1-D model here?

Line 213: 'decade' means 10 years. Do you mean 'order of magnitude'?

Line 211-228: This paragraph run-on, and becomes difficult to follow. Suggest improve the paragraph structure for the benefit of the reader.

Line 233: Suggest alternate phrasing for clarity: "Temperature appears to have a significant impact on atmospheric loss".

Box model

Summary comments: Use of the simple model is a nice way to contextualize the implications of the photochemical modelling work. However, I have some concerns about the parametrizations chosen, and the conclusions thus drawn.

Re original model by Goldblatt et al (2006). Unfortunately, the polynomial fit constants were truncated in the manuscript, but more decimal places are needed. Use p = { 0.0030084, -0.1655405, 3.2305351, -25.8343054, 71.5397861} to reproduce the result shown (I'm sorry about this!). Note also that the value of hydrogen escape coefficient was calculated incorrectly in the original manuscript; the correct value is s = 3.7e-5, but that doesn't have a very big effect (see Goldblatt, 2008, if a reference is needed for that; there is also a bonus chapter on the model there which might be interesting to you).

The original model is modified with parameters to make the methane oxidation rate smaller and the primary productivity bigger. I understand the motivation of the former, but not the latter, given that N is a variable in the original model, not a constant or function. Why not simply talk about increasing N? Results for changing N are presented in the original manuscript, so the result that higher productivity gives more atmospheric oxygen is not novel.

Please be clear about what results came from your 3-D GCM, and which came from your 1-D column model (a 1-D model is not a GCM: do not refer to it as such! See lines 272 & 284 and Fig 15). Note also, line 272, 1-D and 3-D results were shown to be similar, not "identical".

You argue (line 284) that oxidation is faster with interpolated model results, not the parametrization. This does not appear to be strictly true; I think you actually show that steady state oxidation levels (which are essentially what you are showing) are more sensitive to r, where r varies with time over very long timescales. I recall the actual great oxidation in the simple model takes only about 10,000 years.

Please explain why oxygen levels are shown to be constant at low oxygen and high r in Figs 15 & 16. My guess is that this is bogus: that you have used a constant value of your

oxidation rate below 10^{-7} O2, where you do not have model results, which would be erroneous. Either some extrapolation of results is needed, or do not show your results at such low oxygen levels.

You state (line 299) that a reduced methane flux at higher oxygen levels is not treated in the model. This is functionally incorrect, as the methane flux is a very strong function of oxygen via parameters d and g (while the words used in the paper were about organic carbon available to methanogens, and consumption by methanotrophs, the effect is functionally as you seek!).

The realism of the scenario of altering productivity and methane oxidation rate, and the relative timing of these (e.g. Fig 20) need to be justified. What motivates the very long period of high productivity, starting before the glaciations? Why do you show four glacial periods (see, for example, Gumsley, 2017)? In the glacial periods, you keep productivity the same, whereas most people assume that synglacial productivity is much reduced. This is important, because reduced productivity would more than offset the effect of slower methane oxidation.

Figure 18 should be compared to the geological record. Perhaps plot the carbonate record? This gives an opportunity to test your results.

You assert that methane would produce a substantive greenhouse effect, and reduction of this could lead to glaciation (e.g. lines 33, 324, 341), but these comments are not supported. There has been some historical misunderstanding about the strength of this, owing to erroneous results twenty years ago. Recent papers should be consulted, based on which a quantitative estimate can be made of how strong an impact this is (e.g. Haqq Misra et al, 2008; Byrne and Goldblatt, 2014; Byrne and Goldblatt, 2015). I am rather doubtful that the radiative forcing from methane would exceed that from changes in carbon dioxide (not modelled!). I am extremely doubtful that methane would have cause cycles, and have a stronger effect than known cycles or carbon dioxide (e.g. Mills et al, 2011) – though, of course, if you could make the case, then I would be fascinated!

Minor comments

Fig 13: r and Fw are shown with the same line type! Show with different line types or colour.

Line 318: The Archean-Proterozoic transition is defined (presently) by a GSSA at 2500Ma. The glaciations, and the Great Oxidation, are thus Palaeoproterozoic (Siderian) age.

General: you use the terms “over-abundance” of methane or oxygen, whereas I think you simply mean “higher”. “Over-abundance” implies some value judgement, which is not transparent.

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Note: *For abundance of clarity, I'd like to let the authors know that my group has also been working on a paper on temperature effects on the Great Oxidation. A student has been working on this since Sept 2020, and had all their results before I saw your manuscript. Our paper will be submitted in March/April 2022. I have not cross referenced the two manuscripts while reviewing.*