

Comment on acp-2021-406, boundary conditions and constraints?

Anonymous Referee #1

Referee comment on "Influence of atmospheric in-cloud aqueous-phase chemistry on the global simulation of SO₂ in CESM2" by Wendong Ge et al., Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2021-406-RC1>, 2021

General

The paper points to the importance of aqueous iron chemistry in cloud droplets for the removal of anthropogenic SO₂ in the lower atmosphere in a chemistry climate model. There are other CCMs with similar aqueous chemistry and slightly different equations which are mostly cited in the introduction.

It is, however, not clear with which boundary conditions the sensitivity studies concerning Fe³⁺ and the pH are performed, also the definition of 'improved case' is fuzzy and has to be improved. Nevertheless the study is interesting and worth to be published after revision.

Specific

A statement that reactions in liquid aerosol are not included but only reactions in the gas phase and in cloud droplets, is at the beginning of section 2.2. It might be good to have that also earlier, even in the abstract.

Section 2.1: What are the boundary conditions for aerosol? Is dust included or not? Is it related to the iron in the droplets? The provided links are not unique here since there are plenty of scenarios. More details please.

Table 1: Are the chemical equations complete? I wonder about missing HCHO and CH₃CHO and sometimes different products compared to other models. Is HONO in the text and HNO₂ in the table the same? If yes please decide for one notation.

Section 2.2, after line 186 and section 2.3: An initial setting of $[\text{Fe}^{3+}]$ cannot explain how the different scenarios and the spatial distributions are constrained. More information please. Do you mean every time step at cloud formation, if meteorological conditions are favorable for the selected cloud types?

Section 3: In the introduction reactions on mineral dust are mentioned, but not later in connection with the mismatch between model and observations in China, please improve. It might be also useful to include an extra line in Fig 4c with high Fe (e.g. from dust in droplets). Or is this automatically included in China?

Table 2, Figures 4, 6 and 7: The different units are very distracting. Better decide for one common unit and provide the (approximate) conversion factors in the caption of Table 2 or the text.

Section 4, line 344: I suppose these studies are performed with and without the corresponding equations of Table 1. Please mention that clearly if that is the case or explain how you proceeded.

Section 5.1, line 370 (and earlier): it not quite clear how $[\text{Fe}^{3+}]$ at different values is superimposed to the variable values at different locations. It should be better explained already in Section 2 what the "improved case" is with this respect.

Line 376: added to what (and where)?

Section 5.2: Please more details how the pH is entered into the simulations. Is it only via the directly dependent equations or for example via constraining of $[\text{H}^+]$ using Eqns. 33 to 58 of Table 1 in the droplets? Feedbacks with sulfate and nitrate as indicated in section 2.3? Please improve text here.

What is the difference between Fig. S7 (former Fig. 7 in first draft) and Fig. S10? You may skip one because there appears to be almost no difference (except a slightly different caption and differences in Africa for JJA and SON for pH 6). Or explain better in text (section 5 and 2) and the captions.

Technical corrections

Please provide maxima and minima or the range of the color bars in the figures (also in supplement).

Include blanks after ';' in citations.

Line 356, 393: Don't use 'trend' here, wrong word.

In the references often pagenumbers are missing. The doi is provided with 'DOI', 'doi' or nothing before, please use consistent notation.