

Detailed answers are stated below. Black text is the review, blue text our answers.

1. I was a bit confused by the description of the initial aerosol condition and how it connects with the adiabatic parcel vs prescribed LWC modeling setups. The paper states that aerosol (assumed to be completely dissolved in droplets) is assigned to a user specified number of droplet classes. If I understand correctly, in the prescribed LWC scenario the model assumes a mono-disperse distribution of droplets. That would imply that no different droplet classes are needed, as each droplet is of the same size? On the other hand, in the adiabatic parcel scenario the model directly solves the aerosol activation. As a result the liquid droplet sizes should be solved for by the model, rather than prescribed by the user? Could I ask to clarify that?

The droplet size distribution is, indeed, monodisperse when a piecewise-linear LWC is prescribed, distributing the LWC equally among the “droplet classes”. The droplet classes result from the discretized aerosol size distribution prescribed by the user. Thus, the amount of dissolved aerosol is different in the droplet classes, leading to different chemical behavior. This is why multiple droplet classes are made possible. A sentence to clarify this was added to the end of section 2.2 (l.120 in the revised manuscript).

2. Is it also possible to change the default values of equation parameters (like for example water accommodation coefficient in the adiabatic parcel model) through the text files, without recompiling the code? (In the same way as one would change the chemical reaction rate coefficients?) Also, the paper later states that a low value of the accommodation coefficient is used, but I think it is what is typically used. If anything, I saw studies that use lower values.

The possibility of changing the accommodation coefficients via \*.run-file was added in the revised manuscript. See the description of the METEO namelist in the revised supplement (ll. 587-588).

We use `r_alpha` and `r_beta` as relaxation parameters (line 217), as derived in Fukuta & Walter (1970). In this reference, two coefficients are described, one for `r_alpha` and another one for `r_beta`, named the water accommodation coefficient, `alpha_acc`, and the condensation coefficient, `beta_con`.

Note that some authors (e.g., Mordy 1959, Kogan 1991) only use one relaxation parameter, mostly `r_beta` (or a modification). In those cases, `beta_con` is then called the accommodation coefficient `alpha`, instead of condensation coefficient `beta_con`, as done in the original reference. We believe that this inconsistency in the literature caused confusion. Moreover, we believe that our subscript “acc” was misleading. We changed it to `alpha_H2O` and `beta_H2O`, where `alpha_H2O` is what is commonly being referred to as accommodation coefficient (but condensation coefficient in the original reference). This is now also clarified in ll. 218-223 of the revised manuscript.

3. In the equation above equation (6) it should be moist air gas constant?

The density of moist air differs less than two percent from the density of dry air for atmospheric conditions. This is still very important for buoyancy calculations. Since we use a constant updraft velocity and because the density is not substantial for the parcel equations we consider, we chose to stick to dry air formulas for simplicity and conciseness. Depending on further developments or needs, this can easily be changed.

4. It would be great to provide some more discussion and interpretation of what the different patterns in Figures 7 and 8 mean? I admit that I am not very familiar with Rosenbrock methods and I'm wondering what those figures are supposed to convey? Also, why do Figures 7 and 8 appear before Figure 3 in the text?

These figures are almost purely illustrative, but also show little fill-in due to the Markowitz ordering strategy, which is the aim of this strategy. Due to their little scientific value, we removed them and replaced them with a Fig. 8 in the revised manuscript showing some statistics of the presented mechanisms. The new figure conveys how sparsity, fill-in, and computation time increases with the number of species, i.e., the number of equations, in the system.

5. For the readers not familiar with the details of the numerics of Rosenbrock solvers, would it be possible to highlight which parts of the discussion in chapter 4 represent novel approaches, and which parts are standard in the community?

Some clarification was added to the beginning of Section (II. 253-258 in the revised manuscript). The Rosenbrock method itself is standard, but the way it is applied to the chemical systems requires description, even without being novel in the sense of scientific development. The compilation of all numerical developments along with the fast mechanism parser is the novelty of Cminor.

6. In the last column of Table 3 what do 26 (907) and 36 (1800) stand for? Aqueous phase sulfur oxidation should not need this many species and reactions?

The original number of species in the sulfur oxidation mechanism is 26, including all ions, etc. For 50 droplet classes, the species in the aqueous phase exist for every single droplet class, as the concentrations might vary from droplet to droplet. The number of species in the equation system, so to say, is therefore  $n_{\text{gas}} + 50 * n_{\text{aqueous}} = 906$ . The same holds for the number of reactions. We attempted to convey this more clearly in a revised caption of Table 3.

7. What does the green shading represent in figure 4? - I'm guessing it's the effect of plotting blue over yellow with some opacity. But it would be nice to try to keep all three LWC shading regions appear in the same color.

We clarified this by only showing the shading for LWC. The yellow shading for the solar altitude angle was turned into a yellow dashed line in the revised manuscript.

8. Could I ask for a little more discussion of the results presented in Figures 7 and 8? For example: How well do they match the benchmark results from the literature? What was the computation time needed to generate those results and on what hardware? Would it be possible (and would it make sense) to include an example plot showing how the model performance scales with the number of included reactions? How does the performance scale with the number of CPU cores? How the performance of Cminor compare with other models?

The computation times and hardware can now be found in the text (II. 493-494, I. 535, Tables 3 and 4 of the revised manuscript). We also included the performance scaling with the number of species (number of equations in the ODE system) in the new Figure 8. To whether it makes sense to plot performance scaling with the size of mechanisms, please see the comments to point 4 in this document, and II. 558-560. We refrain from discussing efforts to parallelize the Cminor code, scaling with CPU cores etc., as this work has not been started.

In the revised manuscript, we compare Cminor to KPP solving the Master Chemical Mechanism, as now detailed in II. 530-541 and the new Fig. 6 of the revised manuscript. We compare the computation times needed for KPP and Cminor for runs executed on a workstation computer. Shortly: Cminor needs approximately 1.48 times the time KPP needs for the simulation for equal conditions and error tolerances. While KPP has been optimized for years and creates a whole source code perfectly fitted to one specific mechanism (and initial conditions), we are aware of optimization potential left in the basic linear algebra routines of Cminor, and potentially somewhere else. On the other hand, reading and symbolically decomposing the matrix takes 2.2 seconds for Cminor, but it takes 5 hours and 52 minutes for KPP. The KPP code had to be

generated on a comparable Linux machine, because larger mechanisms cannot be handled by KPP on Mac systems (due to restricted stack size limit). Changing a reaction parameter, adding a reaction, etc., always needs this time to be incorporated.

The second comparison to other models is shown in Fig. 7, where our revised manuscript shows the values presented in Jaruga & Pawlowska (2018). Also, the droplet number concentration is discussed and compared shortly to the values of Jaruga & Pawlowska (2018) and the intercomparison study by Kreidenweis et al. (2003) (see II. 546-552 in the revised manuscript).

9. Is the github link missing?

The GitHub link can be found in the Zenodo repository at the end of the page (“Additional Details” > “Software”).