Geoscientific Model Development Discussions

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Reply on RC2

Gwenaëlle Gremion et al.

Author comment on "A discrete interaction numerical model for coagulation and fragmentation of marine detritic particulate matter (Coagfrag v.1)" by Gwenaëlle Gremion et al., Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2020-423-AC3, 2021

We would like to thank the second anonymous referee for the time he/she spent to review our manuscript with very helpful comments that will certainly improve the quality of our work. We include the comments from the referee and our responses. We hope that this version, alongside the improvement related to the first reviewer will meet your expectations for publication.
Sincerely yours,
Gwenaëlle Gremion, on behalf of all co-authors.

- **Bin microphysical models for coagulation are widely used in cloud and aerosol physics. There are many studies that addressed this problem and some excellent reviews (Jacobson, M.Z., 2005; Khain et al., 2015). I would suggest the authors to cite and briefly discuss some papers from these research areas. This can help place the current work in a more general context, and exhibit the advances compared with studies from other fields.**

This comment echoes Reviewer 1's first comment. We do agree that some concepts used in our study come from aerosol physics. We recognize this when we refer to the seminal work of Gelbard et al. (1980) on aerosol coagulation, but we agree that a short discussion on more contemporary work in this field is relevant and will be added. We thank the reviewer for its suggestion.

- **In Eqs. (8) and (9), the triplet operator that represents both coagulation and fragmentation for a given bin, should be discussed in more detailed. It is clear from Eq (9), that the increase in the number of particles in bin k is proportional the product of particles number concentrations in bins i and j. However, the coagulation and fragmentations rates (coagulation kernels) from Table 2 are considered constant, and not depending on particle radius, chemical composition or terminal velocity of the particles.**

Coagulation and fragmentation rates depend on particle size through a number of different processes and our model takes this into account. To better reflect this, we have modified the equations describing our model (mainly Equations 8-9) so that they use size-dependent coagulation and fragmentation rates, and we briefly summarise how these rates depend on size, citing relevant literature. It is only when we design the numerical experiments that those rates are set constant, to facilitate the interpretation of the results and the assessment of robustness to resolution and discretisation.

- **The mechanisms for particle coagulation are not emphasized or discussed. For example, in Jackson (2001) three mechanisms for particle coagulation are discussed: Brownian diffusion, shear (laminar and turbulent), and differential sedimentation. It is not clear if coagulation and fragmentation rates are considered constant just to check the performance of the algorithm, or as some kind of approximation for different physical processes like differential sedimentation.**

We agree with the reviewer that it was not clear from the manuscript whether the model was only applicable with constant rates and whether or not we recognized that there are well-known mechanisms and well-described formulations that exist. In response to the previous comment, we will revise the model formulation by adding size-dependent rates, including coagulation. Shortly after, we will recall the mechanisms driving particle collision and coagulation, namely Brownian motion, shear and differential sedimentation. It is only when we describe the numerical experiments that we will set these rates to constant values and say why we choose to do so.

- **In page 14, line 218, it is written that "Coagulation of particles belonging to bins 1 μm and 10 μm would ideally produce particle size 11 μm", which is in general not true for the radius of the resulting particles after coagulation.**

We are thankful that this point was raised, as we did not precise, indeed, that this rule applied when considering size as the particles' volume. We will correct this statement by referring to volume (in μm^3) instead of the one-dimensional size (in μm).

- **In the discussion of simulation results, authors stated that "coagulation leads to a reduction of Cp in small size bins and an increase in larger ones for both LR and HR, resulting in a linearly increasing distribution of Cp over the resolved size range". And "fragmentation yields a reduction of Cp in larger size bins to the benefit of an increase in the small ones", as in general expected. However, it could be interesting to check further the performance of the model for the coagulation case only, by comparing the results obtained from the kinetic equations developed by the authors with analytical solutions of the Smoluchowski equation for a constant coagulation kernel (for example).**

Good point, thank you. We made a formal comparison between Smoluchowski's approach and ours that will be presented in the revised version. In essence, there exists very few differences between the two. If we put aside the closure for the unresolved range, the only difference resides in the fact that Smoluchowski's formulation is in terms of number of particles, while ours is in terms of concentration. This slightly modifies the evolution equation since the total concentration is conserved for a given reaction in our setup while the total number of particles is not conserved in Smoluchowski's (two particles are combined to yield a single new one). Nevertheless the two formulations are equivalent and, in this context, it is difficult to imagine a setup that would allow a comparison outside of a simple bookkeeping between concentration and number of particles.