

Author's response for MS No.: gmd-2020-423, Gwenaëlle Gremion et al.
"A discrete interaction numerical model for coagulation and fragmentation of marine detritic particulate matter"

TOPICAL EDITOR

Dear Mr. Arabas

Thank you for the editorial review of our submission. Please find below a point-by-point response to the reviews including a list of the relevant changes made in the manuscript.

Thank you for your consideration, do not hesitate to contact me for any further requirement,

Best Regards

Please note that the page and line numbers refer to the *Author's track-changes file* submitted alongside this *Author's response*.

Minor comments

The CC licenses are discouraged for use with software (<https://creativecommons.org/faq/#can-i-apply-a-creative-commons-license-to-software>), please consider releasing the source code under a software license

We are thankful for the recommendation, as we were not really familiar with the licence regarding software. We modified the licence from *Creative Commons Attribution 4.0 International License (CC BY 4.0)* to *GNU General Public License v2.0 or later*, and specified it in the *code availability* section :

The code concedes to the GNU General Public License v2.0 and is written in Fortran 90 and requires the gfortran compiler.

The v.1 version specification introduced in the title seems not to be reflected in the repository files, metadata or the zenodo archive, please add the v.1 version number to the repository (git tag?) and create a zenodo archive that includes the version number

We are surprised that the specification is not clear, as the version number is associated to the DOI in the zenodo archive and specified as reflected in the citation used. However we made an adjustment as the word 'version' was written twice in the first citation used. The current citation will be such as :

Gremion, G. and Nadeau, L.-P.: Source code and user manual of the Coagfrag Model (Version 1), Zenodo, 2021-01-11, <https://doi.org/10.5281/zenodo.4432896>, 2021

To avoid any confusion, we displayed also the entire word *Version* in the title of the article too :

A discrete interaction numerical model for coagulation and fragmentation of marine detritic particulate matter (Coagfrag Version 1)

Representing cloud physics myself, I concur with the reviewers that highlighting links with this domain sounds very appropriate; however, the introduced changes seem somewhat cursory. On the one hand, coagulation/fragmentation models are used in multiple other domains - not only cloud and oceanic modelling. On the other hand, several of the specific steps in the model formulation presented can be linked with works from cloud physics. Please consider mentioning links with other domains where coagulation/fragmentation models are applied. For example, in Pego (2007) the following applications are mentioned: "microdroplet formation (in clouds, ink fog, smoke, fuel, paint, etc.), the kinetics of polymerization, hashing algorithms, and the clustering of colloids, phytoplankton in "marine snow," planetesimals in stellar accretion disks, and stars themselves" - just not to create a feeling that oceanic and atmospheric modelling are considered the only ones worth mentioning [...].

We agree that we can indeed reinforce the fact that coagulation/fragmentation are used in other fields and we modified the text accordingly, based on your suggestions. Here is the modified text (p.2 line 62):

We note that coagulation and fragmentation of particles is a natural phenomenon that happens in a very broad variety of situations. It has been studied in many disciplinary fields, including atmospheric sciences, especially in microdroplet and cluster formation (e.g. Pruppacher and Klett, 2010), but also in chemistry (e.g. Lee et al., 2018), astrophysics and engineering (see the review of Pego, 2007). In oceanography, it is also applied to aggregation of nanoplastics with colloids (Oriekhova and Stoll, 2018) or the oil-marine snow interaction (Dissanayake et al., 2018; Burd et al., 2020).

What concerns cloud physics, do I understand correctly that, e.g., the Appendix B in Tzivion et al. 1987 [...] is relevant when discussing eq. (4)? Pointing out such links with other domains would certainly be beneficial for promoting your work in the respective communities.

As we understand, Appendix B in Tzivion et al. (1987) refers to moments of the particle size distribution function, while our paper model spectral interactions without inferring any underlying or a priori distribution function. Equation 4 is an empirically-based function that relates the elemental (carbon) content of particles to their volume. However, what we try to solve is the volume-dependent concentration in time. In short, it is not relevant to discuss Tzivion et al. here, although we really appreciate the suggestions made to try and promote our work to other communities. This being said, we modified slightly Equations (1) and (5) to highlight the time-dependence of spectral variables C and n , so that the problem we seek to solve is more clearly posed.

We also added a sentence in the introduction that clearly state what distinguishes our approach from existing ones, which will also clarify the meaning of discrete in the title and in the abstract. Altogether, these changes makes it clear now that we discretize particle concentrations into size bins and solve the evolution in time of these size-dependent concentrations in an Eulerian numerical framework. Here is the modified text (p.3 line 84):

Our approach differs from the so-called sectional approach of Jackson and Burd (2015) in that the discretized size spectrum we use is an integral quantity that depends on the discretization, as opposed to a spectral density.

On a related note, when referring to the Smoluchowski equation, it is worth to clarify that the original formulation had not featured breakup. For example, in Hansen 2018 [...] the form with break-up terms included is labelled as "generalized Smoluchowski equation".

Thank you for pointing it out this nomenclature, we made the appropriate adjustment in p.12 line 202 :

Focusing on the resolved range only, Eqs. (16) and (18) can be combined to yield a discrete version of the generalized Smoluchowski equation (e.g., Smoluchowski, 1916; Hansen, 2018)

Nomenclature issue: already in the abstract, it is mentioned that the framework is based on "discrete size spectrum" which can be interpreted as sampled at discrete points (as is done in probabilistic formulations of coagulation models). Here, a size range is associated with a "bin". It seems worth clarifying - discretised (into bins) vs. discrete?

See answer to previous comment.

Also, a mention of probabilistic (Monte-Carlo) alternatives pointed out by Referee #2 would be valuable in my opinion (perhaps the recent GMD oceanic-modelling paper by Jokulsdottir & Archer[...]).

We explicitly noted the existence of Lagrangian approaches and the work Jokulsdottir & Archer (2016), making it also clear that we propose a Eulerian model and why we do so. Here is the modified text (p.3 line 67)

We note also that there a variety of modeling approaches, including Lagrangian formulations with stochastic processes (e.g. Jokulsdottir and Archer, 2016). However, Eulerian formulations are those that are still best applicable to OGCMs-BGCs and that will be considered more specifically here. The present work stems from numerous Eulerian modeling studies, most of which are ...

The "three particles" wording seems misleading as coagulation involves two particles and fragmentation - as modelled here - also does not feature three particles at any given time (one before, and two afterwards, right?)

Coagulation and fragmentation are fundamentally involving three particles (one before and two after for fragmentation, and two before and one after for coagulation). This is what we describe in Figure 2 and this is how our reaction terms are defined, based on indices (i,j,k) .

To avoid further confusion, and to make the model framework even more general and coherent, we modified the fragmentation rate \mathcal{F}_k that depended only on k , to \mathcal{F}_{ij} so that it may depend more generally on particles i and j , recalling that i , j and k are linked by the additive rule $V_i + V_j = V_k$. This allows embracing a larger space of possibility in the final distribution of particles size resulting of fragmentation, that may not be (in certain conditions) equal over the size range.

We therefore modified the fragmentation rate expression from \mathcal{F}_k to \mathcal{F}_{ij} in Equations (9) and (22) and by \mathcal{F}_{ip} in Equations (19) and (20).

Please mention that Matlab is required to reproduce the analysis using the scripts provided in the zenodo archive;

We added the following mention in the *Code availability section* :

Matlab 2015b minimum is required to reproduce the figures using the scripts provided in the zenodo archive.

Please provide all figure files in vector graphics format (e.g. saving to pdf instead of png when plotting)

I sincerely apology, it was an oblivion from my part. I thought they were submitted in a PDF format at a previous step of the submission process. In addition as no modifications were required after referees revision I did not think to upload them again. Please find them properly attached this time in a PDF format in the submission form.

Technical/editorial points:

- *Spell "Fortran 90" not "fortran90"*
- *For the Smoluchowski reference, this seem to be more of a permanent link.: (BTW, here is the other part of the article)*
- *The page range for Smoluchowski reference should be: 557-571*
- *Colon instead of dash in the title of Doney et al '96?*
- *More precise DOI for Doney et al.2003*
- *Correct DOI identifier for Le Quéré et al*
- *Correct DOI identifier for Zahnw et al.*

We are grateful for this detailed verification. We made the changes accordingly to follow the seven mentioned points.