

Review of “Stochastic coalescence in Lagrangian cloud microphysics?” by Dziekan and Pawlowska

Super droplet (SD) methods (SDM) are a novel and promising approach in cloud physics. Generally studies dealing with SD methods are welcome to better understand and gain experience with this type of model class. The present manuscript specifically addresses the coalescence process and compares a specific SD algorithm with other approaches like DNS, bin models or analytical derivations.

My impression is that the work is in general suitable for publication in ACP, as many interesting tests have been performed with a specific SDM.

Nevertheless the manuscript needs major revisions.

The presentation is too short to fully understand what has been done and to be able to judge it.

Moreover, the statements are too general. Also the motivation behind choosing the presented tests must be made clearer. In the present style the presented tests resemble a bit a random collection of tests related to a specific SD coalescence algorithm.

General points

1. The description of your method and results is too short and often not clear enough. For a reviewer it is difficult to understand what you have done in detail and this makes it hard to thoroughly rate your work. The description in section 2 must be considerably expanded and be more precise. Also the results section should be improved. For example the motivation behind showing the comparison in section 3 is not really clear to me.

As an example I go over page 3 and try to highlight what I miss there and where I suspect that other readers would get stuck:

- It is not always clear if you talk about real droplets or super-droplets. It should be always clear if your statement relates to the real world or the super droplet world.
- You should define the coalescence probability of a SD pair.
- Can collections occur between droplets in one SD?
- I.9: Do you use two types of simulations or is it only the initialisation that differs between the two types? Then I would not call it “types of simulations”.
- In general I can imagine how the “constant SD” initialisation works, however I am confused by your description.
 - I.21: do you mean large or small N_{SD} ? Or large r ?
 - r_{min} and r_{max} are defined by the relation in line 18. Using the $\Delta \ln(r)$ definition of line 19, you end up with implicit equations in the two variables. I am pretty sure this is not what you wanted to say.
 - You initialise additional SDs to better represent the tails of the SDs. Adding those SDs to your ensemble, isn't it necessary to reduce the multiplicity of the SD drawn from the largest bin? Is the refinement done at both sides? In the end, the actual number of SDs should be higher than the nominal value N_{SD} ? How much higher? Is the one-to-one initialisation the limiting case of the constant SD initialisation? Are the multiplicities in the constant SD approach integer values? How is the rounding done?
 - I.20: To be more explicit, you should write that one SD is created per bin and its radius is randomly selected.
 - I.23: Do you want to say that the probability *is allowed* to exceed 1. Why does this occur only here, and not in the one-to-one simulation? Is the time step longer? Why don't you reduce it then in this case?
 - What are multiple collections?
 - Do you use a constant time step throughout a simulation?

2. Your conclusions are too general. Your paper reads like a general comparison between the one and only SDM approach and all kinds of other algorithms.

Coalescence (or similarly coagulation of aerosols and dust or aggregation of ice crystals) can be treated in many ways in particle-based approaches (see algorithms by Andrejczuk et al, Shima et al, Riechelmann et al, Sölch & Kärcher, Zsom & Dullemond, Kolodko & Sabelfeld, deVille et al). There is not the one natural way to do this. Similarly, various algorithms exist for bin model approaches.

Please make clearer which statements hold in general and which are probably only valid for your specific SDM.

A recent study by Unterstrasser et al compared three different SD algorithms for the collection process (your all-or-nothing SDM is among the tested algorithms). Each algorithm has its strengths and weaknesses. One major finding was that the performance depends strongly on how the SDs are initialised from a given size distribution. This has several implications: 1. an accurate description of your initialisation is needed (see point 1) and 2. Are your simulations sensitive to initialisation details besides the number of SDs?

3. In my opinion you present five types of tests: 1. Comparisons with algorithms for the master equation (ME), 2. Comparisons with DNS algorithms 3. Comparisons with algorithms for the Smoluchowski equation (KCE) 4. Comparison with analytical results and 5. Stand-alone sensitivity tests of your SD algorithm.

With each type of test different aspects of your SD method can be tested. Each reference model you compare with (Bott, Alfonso, Onishi, Kostinski & Shaw) differs in which physical processes are explicitly treated. You often miss to clearly specify the purpose of and the motivation behind the individual evaluation steps you take. This must be made clearer in the revised version.

4. Your study is written in a style that implies that your SD algorithm does not solve the KCE. By comparing your SD results with KCE results you seemingly disclose shortcomings of the KCE description.

In fact, SDMs also rely on KCE and your study is not really suited to question the physics of the various formulations. In my understanding, you compare different numerical strategies of solving the KCE.

The probabilistic nature of your SDM is inherent to your specific algorithm. The SDMs of Riechelmann or Andrejczuk are not probabilistic. On the other hand, I agree that the probabilistic component of your SDM looks like it attempts to mimic the processes in nature. Nevertheless, the two should not be mistaken. In the superdroplet world of your SDM, the probabilistic approach comes from the fact, that each superdroplet represents a large number of real droplets and you may or may not perform a superdroplet collection. This not per se related to the stochastic nature of the real world processes that accounted for in the master equation.

Major points:

5. In my understanding there two mathematical descriptions of the coalescence process: The Smoluchowski equation and the master equation where only the latter accounts for correlations. You never state it explicitly but I suppose that your SD method is based on solving KCE.

Many spectral bin methods exist for the KCE and in the recent past SD methods for KCE were introduced. Hence, demonstrating agreement between your KCE solver and the ME solver by Alfonso is only reasonable for a physical problem where correlations are negligible.

If you want to show the numerical consistency of your approach, then a comparison with

other well-established KCE solvers would be more straightforward. Could you give reasons why you compare results of your KCE solver and an ME solver? Or do you want to claim that SDMs implicitly account for correlations?

6. I am not exactly sure what you intended to show in section 3. Did you want to demonstrate the suitability of your linear sampling of droplet pairs? Then you should compare results of your algorithm, once with linear sampling and once considering all possible combination. For a simulation with 30 droplets (as done in the comparison with Alfonso) this should be feasible. How do the curves in Fig.3 and 4 change, if you evaluate all possible combinations instead of linear sampling (at least for $N_0=10$ and 100)?
7. Is it all reasonable trying to sample a continuous exponential distribution with 10 SDs? Are the total mass and number of the SDs (averaged over all ensembles) equal to the prescribed values? What about the higher moments, do they match the values of the analytical distribution? This is an important aspect as much of your evaluated variability may come from the initialisation and not so much from “stochasticity” of the SDM.
8. Even though Fig.4 shows simulations with an initialisation analogous to Onishi, the presented test is a stand-alone test (following the above categorisation). Hence, further tests with other kernels or other initial size distributions can be made (as no comparison with Onishi is required) in order to corroborate your findings about how many SDs are necessary to reach convergence.
9. In Fig.4 and following figures, does the Smoluchowski line depend on the parameter choices of the underlying Bott algorithm (time step or number of bins)? Bott is known to be diffusive; this may explain the faster generation of large droplets. Anyway I would not call it the Smoluchowski line, it is the Bott line. The line may look differently for other bin KCE algorithms. Moreover, your lines are also “Smoluchowski” lines (see general point 4).

Minor points:

10. p.3, l.21: Is the sol-gel transition an important aspect in cloud physics? You note that mass conservation is not guaranteed for some kernels. Are those kernels relevant in cloud physics? In super-droplet approaches mass conservation should be guaranteed by construction.
11. I do not understand the statement “the number of collision pairs is reduced” in p.4 l.4.
12. The paragraph starting p.4 l.11 should be moved to section 2.
13. For Figs.1 & 2 it would be ideal to obtain the data from Alfonso and include it in the plots.
14. P.2 l.13: Tanaka & Nakazawa present solutions for kernels other than the constant kernel. See also Table 2 in Alfonso, 2015.
15. P.5 l.5. Isn't this statement trivial? Probably any algorithm for KCE is faster than solving the master equation. A comparison among various KCE solvers would be fairer.
16. Figs. 2&3 show relative standard deviation of the largest droplet mass. Wouldn't it be interesting to know how large the largest droplet mass is? How many collections have occurred to form the largest droplet?

17. P.7 l.10-12: I am confused. DNS simulations compute droplet trajectories and directly evaluate if there are collisions between droplets. Why do you need a coalescence kernel in this numerical approach?
18. Fig.8: Do you also use the 20um cut-off in the Bott simulation? It is not explicitly stated in the text.

Technical points:

- Figure caption should include the information “t=2500s”.
- P.5 l.9: droplet, not dropeltS.

References:

M. Andrejczuk, W. W. Grabowski, J. Reisner, und A. Gadian. Cloud-aerosol interactions for boundary layer stratocumulus in the Lagrangian cloud model. *J. Geophys. Res.*, 115:D22214, 2010. doi: 10.1029/2010JD014248

R. DeVile, N. Riemer, und M. West. Weighted flow algorithms (WFA) for stochastic particle coagulation. *J. Comput. Phys.*, 230(23):8427–8451, 2011. doi: 10.1016/j.jcp.2011.07.027.

A. Kolodko und K. Sabelfeld. Stochastic particle methods for Smoluchowski coagulation equation: Variance reduction and error estimations. *Monte Carlo Methods and Applications*, 9 (4):315–339, 2003. doi: 10.1163/156939603322601950

T. Riechelmann, Y. Noh, und S. Raasch. A new method for large-eddy simulations of clouds with Lagrangian droplets including the effects of turbulent collision. *New Journal of Physics*, 14(6):065008, 2012

S. Shima, K. Kusano, A. Kawano, T. Sugiyama, und S. Kawahara. The super-droplet method for the numerical simulation of clouds and precipitation: a particle-based and probabilistic microphysics model coupled with a non-hydrostatic model. *Q. J. R. Meteorol. Soc.*, 135(642): 1307–1320, 2009.

I. Sölch und B. Kärcher. A large-eddy model for cirrus clouds with explicit aerosol and ice microphysics and Lagrangian ice particle tracking. *Q. J. R. Meteorol. Soc.*, 136:2074–2093, 2010.

H. Tanaka und K. Nakazawa. Stochastic coagulation equation and validity of the statistical coagulation equation. *Journal of Geomagnetism and Geoelectricity*, 45(5):361–381, 1993. doi: 10.5636/jgg.45.361. URL <http://doi.org/10.5636/jgg.45.361>.

S. Unterstrasser, F. Hoffmann, und M. Lerch. Collection/aggregation algorithms in Lagrangian cloud microphysical models: rigorous evaluation in box model simulations. *Geosci. Model Dev.*, 10(4):1521–1548, 2017. doi: 10.5194/gmd-10-1521-2017.

A. Zsom und C. Dullemond. A representative particle approach to coagulation and fragmentation of dust aggregates and fluid droplets. *Astronomy and Astrophysics*, 489(2):931–941, 2008. doi: 10.1051/0004-6361:200809921.