GMD manuscript #2020-404: reply in the third round of review

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January 2022

We hereby express our appreciation for the reviewer's feedback which we followd point-by-point revising the text. Below, we include replies to all points. Quoted text of the review is typeset in teal and with larger margins.
A revised manuscript with changes automatically highlighted using the latexdiff tool is enclosed with additions marked with blue colour and deleted text in red. Additions to the bibliography are not colour-highlighted, but all references to new bibliography items are within blue-underlined blocks in the text.

comments by Anonymous Referee #4, 01 Dec 2021

> General comments:
> 1. The authors have improved the presentation of the manuscript substantially in this revision. However, it is still hard to read. It took me more time to understand and comment on the writing instead of science. I suggest all the authors read through the manuscript carefully to improve the readability. I would also encourage the authors to explain each figure clearly and logically. Please see my suggestions in the section of specific comments.

We have revised the manuscript following the provided suggestions. Additionally, numerous language corrections aimed at improving flow in the text were introduced.

> 2. It is still unclear to me what the advantage of using the upwind scheme over high-order schemes is. How is the computational cost of this scheme compared to the high-order schemes? Discussing this briefly in the introduction and the discussion part can be beneficial for the community.

MPDATA is a higher-order scheme based on upwind. The advantage of basing the scheme on upwind is that MPDATA retains the salient features of upwind: conservativeness, small phase error, sign preservation. This is now mentioned in the very first paragraph of the paper.

Indeed, in the result section, the authors argue that "...As a result, the algorithm is characterised by reduced numerical diffusion while maintaining the salient features of the underly...". Which benchmark scheme did you compare with?

Upwind, clarified.

3. The authors found that "...even a tenfold decrease of the spurious numerical spectral broadening can be obtained by an apt choice of the MPDATA variant (maintaining the same spatial and temporal resolution), yet at an increased computational cost...". In my opinion, this is an interesting finding since it helps understanding the artificial broadening of particle-size distribution. What is the benchmark for this conclusion?

The benchmark behind the "tenfold" figure is the upwind solution. This has been clearly indicated in the discussion of Figure 9 based on which the statement is made. The passage in the abstract which the Referee refers to is now clarified, and the sentence reads: "*... compared with upwind solutions, even a tenfold decrease ...*".

I am not asking for performing more simulations. Comparing your current results to some references should be enough to address the question.

Throughout the paper, the results from numerical simulations with MPDATA are compared to both analytical solutions (box test case), as well to upwind numerical solutions (box and single-column test cases).

4. Is the "box model simulation" direct numerical simulation? What is your numerical setup? Is it a 1-D case driven by a constant supersaturation? What are the governing equations of the motion of particles? How do you determine your timestep? What are the boundary conditions?

The "box-model" notion was used here as in the chemical/microphysical jargon meaning a model with no spatial dimension, without any fluid flow. Particle positions or motion are not considered at all. The only "flow" is in the size-spectral dimension. The boundary conditions are specified in the text: *linear extrapolation is applied for G, while both ψ and GC are set to zero within the halo*. For the sample simulations discussed in the main text, the timestep is set to $\Delta t = \frac{1}{3}$ s as indicated in the text, while a range of timestep settings is used to perform the convergence analysis presented in the appendix.
To avoid confusion with DNS, the lack of spatial dimension is now verbosely stated in the text: both in the abstract and near the first mention of a box-model problem.

5. What is the link between the "box model simulation" and the single-column model? Shouldn't the results from "box model simulation" be used or compared to the sub-grid scale modeling of large-eddy simulations before jumping to the single-column model? Can the conclusion of MPDATA from the box simulation

be carried over to the single-column simulation? I encourage the authors to discuss this link in depth, which can be a highlight of this study. Again, I cannot recommend the publication in its current form. A major revision is required for further consideration.

Assuming the above comment is based on the assumption of the box model being a kind of direct numerical simulation, let us reiterate that there is no physical motion of any kind considered in the box test case. The single-column setup adds the spatial dimension to the problem. All conclusions concerning spectral advection and spectral broadening carry over to the spatio-spectral problem of the single-column simulations.

Specific comments:
1. P1, L5: Could you please rewrite "The numerical diffusion problem inherent to the employment of the fixed-bin discretisation in the numerical solution of the arising transport problem is scrutinised." to make it more concise?

The first sentences of the abstract were rewritten.

2. P1, L5: What is "carried out"? Neither "Eulerian modelling approach" nor "evolution of the probability ..." fit the subject.

Changed to: "*a fixed-bin discretisation (so-called "bin" microphysics) is used in solution ...*.

3. P1, L25: What is a "The single-column problem"?

Rephrased to "*single-column test case*".

4. P1, L51: What is "a population-balance equation"? Please add references. Isn't it the Boltzmann transportation equation conserving mass?

Given that the present work deals only with the condensational growth of a population of particles, a reference to Boltzmann transport equation seems to add little to the presented discussion. While not recalling the connection with Boltzmann formalism to be prominently featured in any of the cited references, let us note that the term "population-balance equation" had been featured even in the title of Tsang & Rao (1990) for describing the very same problem and even the very same numerical solution methods. We thus intend to leave it as is. A reference to a textbook on population balance equations (Ramkrishna 2000) is now added right after presenting eq. 1.1.

5. P2, L10: Do you mean "turbulent mixing"? Numerical approach?

This sentence was meant to juxtapose mixing (physical) effects with numerical solution artefacts. It is now split in two and augmented with more examples of physical processes (turbulent mixing, diverse particle composition, radiative heat transfer effects), with reference to discussion in Feingold and Chuang (2002).

6. P2, L15: Please be more specific about the challenging physical processes. What is “represent the subtleties”?

Added the following: ”*which link the physio-chemical properties of single particles with ambient thermodynamics through latent heat release and multi-particle competition for available vapour*”.

7. P2, L20: Please cite “https://doi.org/10.1146/annurev-fluid-011212-140750”.

This work had already been cited two sentences ahead. All reference parentheses in this introductory paragraph have the ”e.g.” disclaimer.

“inherent limitations” of what?

Inherent limitations of ”discretisation”.

8. P2, L35: in determining both the ...

Corrected.

9. P2, L40: Please add references to the statement “The parameterisations used in climate models are developed based on smaller-scale simulations resolving particle-size spectrum evolution.”. Small-scale models can simulate the cloud microphysical processes while GCMs cannot. Can you give an example on which GCM adopts processes simulated using which small-scale model?

Representation of cloud condensation nuclei activation in GCMs can be a good example here. Simple parameterisations for use in GCMs are built using detailed parcel-model simulations involving representation of droplet size-spectrum dynamics. A mention of it is now added to the sentence.

10. P2, L75: What is “title =”? What do you mean here?

This was an accidentally included part of a bibliography record – removed.

11. P2, L105: droplets?

Changed ”numerical broadening of the spectrum” into ”numerical broadening of the cloud droplet spectrum”

12. P3, L5: by comparing to ...

A sentence explaining that the study compared upwind to an Eulerian-Lagrangian schemes is now added.

13. P3, L5:the upwind ...

Added ”the”.

> 14.P3, L25: praised. What do you mean by “prediction accuracy of...”?

The word ”accuracy” is now removed (as it was indeed not used in the cited work).

> 15. How do I connect the paragraphs above and below the paragraph “Aerosol Science: ...”? What is the scientific question you want to summarize from this book?

The literature review is presented in chronological order, which is why the reference to Williams and Loyalka 1991 book is given at this point – after Tsang and Rao 1988, and before Kostoglou and Karabelas 1995). The book lists MPDATA among methods (of choice) for solving the condensation term in aerosol population balance equations, which is the reason for citing it here.

> 16. P3, L40: I don’t understand this sentence. Please rephrase.

Rephrased and shortened.

> 17.P3, L45: fixed and moving bin-approaches

Rephrased.

> 18. P3, L50: What do you mean by “...at.., ...at...”?

The entire passage is now rewritten.

> 19: What do you mean by “a grid composed of 2000 size bins”? Is it the spatial resolution?

Spectral resolution. Rephrased to: ”*spectral discretisation involving 2000 size bins*”.

> 20: P3, L90: I don’t understand the statement of “there is a degree of freedom in the choice of the particle-size parameter used as the coordinate”. n(r), n(s), and n(v) are exchangeable. It is a matter of preference of using the radius binning or mass binning. How is it related to “a degree of freedom”? The same comment applies to “p(r(x))”.

By ”degree of freedom” we meant ”it is a matter of preference”, yet since the choice influences the numerical solution characteristics, we would also refrain from calling it just ”preference”. The two passages are now rephrased and start with ”one has the choice” instead of ”there is a degree of freedom”.

> 21: P4, L20: The sentence is incomplete.

Corrected.

> 22: Caption of Fig.1: What is "$ln2(r^3)$"?

This is the definition of the mass-doubling grid layout, what is now verbosely stated in the figure caption and the defining equation is given in parenthesis.

> To improve the readability of Fig.1 and 2, you could move the title to the y-axis and use the abbreviation "m, cm, um" instead of words. Please check all the figures and improve the labels and units presented in them.

Figures 1 through 8 were re-plotted with abbreviated unit labels.

> I still don't understand the purpose of showing both Fig.1 and 2. Fig.2 looks almost identical to Fig.1. If you want to compare the two cases, you should plot them in a same figure.

Both figures include spectra at t=0. These are discretised on different grids – this is the difference between the two figures and the purpose of having both presented in the paper. Merging the two figures would cause the two t=0 histograms to overlap and be illegible.

> 23: P5, L10: Which figures are you talking about? This paragraph is repeating what is said in the caption of Fig.1. What is the point of repeating it?

Removed.

> 24: P5, L15: What do you mean by saying "integrating the number conservation law"?

Rephrased to "*solving number conservation equation*".

> 25: At least the last three paragraphs of section 2.2 can be merged into one. You may describe and explain the results in a logical way. This is just one example, please carefully read through the description of other figures and make the storyline fluent and concise.

Merged and augmented with clarification of linear vs. mass-doubling grid comparison.

> 26: P6, L5: Which "resulting in" which?

Rephrased to "*what results in*", "*which can be further ...*"

> 27: P6, L10: What is "sought modified equation"?

In the modified equation analysis outlined in the paragraph in question, one seeks the partial differential equation that is actually represented by a numerical scheme (instead of the original physical equation). In this case, the original physical equation is the advection equation, while the leading terms of the numerically realised modified equation constitute an advection-diffusion equation. The additional diffusion term originates from numerical approximation, hence the term "numerical diffusion".
To clarify the statement, the following sentence is now added at the beginning of the paragraph: "*In a nutshell, the analysis involves: (i) Taylor-expansion of each term of the numerical scheme, (ii) elimination of higher-than-first order time derivatives using the time-differentiated original advection equation, and (iii) derivation of a partial differential equation, referred to as the modified equation, that a given scheme actually approximates in lieu of the advection equation.*"

> 28: P6, L55: What do you mean by "transported signal" and "variable sign signals."? Numerical formula. Please rephrase this sentence. The grammar is not correct.

Split into two sentences, replace "transported signal" with ψ, removed "numerical". Also, the term "signal" was replaced with "field" elsewhere.

> 29: P6, L65: About this statement "Overall, while the MPDATA solutions are superior to upwind, the drop in amplitude and broadening of the resultant spectrum still visibly differs from the discretised analytical solution.", is it because of the hyper-diffusion method used in MPDATA or the bin resolution?

Nowhere in the present work, we have used the term "hyper-diffusion". The corrective iterations of MPDATA employ anti-diffusive velocities. The corrections reduce the drop in amplitude. Of course, the bin resolution influences the results, yet in the passage in question, we compare MPDATA and upwind solutions obtained for the same bin resolution.

> The upwind scheme presented in Fig.1 of "https://doi.org/10.1002/2017MS000930" also underrepresents the amplitude of peaks.

Reference to Fig 1a in Li et al. 1997 is now mentioned as well.

> 30: P7, L5: What do you mean by "linearising MPDATA about an arbitrarily large constant"? It should be "background scalar field".

The employed wording is taken from Smolarkiewicz 2006 (also used in Hill 2010). The requested "background scalar field" had already been used in the parenthesis in the very same sentence.

> 31: P7, L15: "..., such". It should be a new sentence "Such ...".

Rephrased and split in two sentences as suggested.

32: You can combine Fig 1, 2, 3, and 4 into one figure to improve the readability. Please go through the manuscript carefully and make the figures concise.

Figures 1–8 may certainly appear repetitive, yet this stems from the tutorial character of section 2. Moreover, the discussed features of numerical solution such as: differences in employed grids, appearance of negative values or differences in bin amplitude for different number of MPDATA iterations would be obscured if plotted all on a single figure.

33: P7, L25: Are the "negative values" generic of the "infinite gauge" or just for your case? Please explain why they are negative.

The previous paragraph ended with "*such gauge choice decreases the amplitude of the truncation error, however, it makes the algorithm no longer positive definite.*" The above sentence was split in two leaving the statement on lost positive-definite property clearer.

34: The last 3 paragraphs in the section 2.11 can be merged into one.

Merged.

35: P10, L10: "right panel" → "rhs panel". Please check "right" and "left" expressions all across the manuscript.

In all references to figure panels, "righ-hand panel" and "left-hand panel" are now used.

36: P10, L20: "so" → "such that"

Corrected.

37: P10, L25, L30: I don't understand this paragraph. Please check the grammar.

The first long sentence was split in two. A reference to more comprehensive discussion of the issue was added (Smolarkiewicz and Rasch 1991).

38: P11, L10: "what" → "that"

Corrected.

39: P11, L55: What is the "Ordinary particle volume concentration"?

It was meant to underline difference of per-volume concentration vs. specific number concentration (per mass of dry air). The word "ordinary" is now removed and the sentence starts with: "Particle volume concentration (as opposed to specific number concentration)...".

40: P12, L30: Is "w1 "the initial vertical velocity?

No, as had been stated in the very same sentence, w_1 is a parameter of the equation determining the time evolution of the vertical momentum density: $\rho_d w(z,t) = \rho_d w_1 \sin(\pi t/t_1)(1 - H(t-t_1))$.

41: P12, L75: How is the vertical velocity determined?

To clarify, the equation defining the vertical velocity is now numbered (3.1) and referenced.

42: The caption of Fig.10 does not read right.

Rephrased.

43: The first paragraph of section 3.3 describes the numerical setup. It can be moved up to the one-sentence paragraph.

Moved.

44: Fig.11: It is hard to distinguish different lines in the vertical-profile plots. Can you use different symbols?

The different lines are now plotted with different colours in addition to different line styles.

Why does “MPDATA iterations: 1” yield different d compared with “MPDATA iterations: 2” and “MPDATA iterations: 3”.

This is the key message of the paper. The relative dispersion d is the measure of spectrum broadness. MPDATA corrective iterations reduce numerical broadening yielding smaller d.

45: P13, L40: “the only conclusion here is that the visualisation method used in Fig. 10 is apt to highlight this feature”. This statement again questions the application of the single-column simulation in this manuscript.

This statement was indeed unfortunate, and is now replaced by one ending simply with ... *no physical interpretation is warranted*. The single-column KiD framework is certainly very simple, yet it has proven in numerous cited works to be a useful model for works focusing on the basics of cloud microphysics/macrophysics interplay - as it is used herein.

I still don’t understand if the conclusion about the MPDATA from the box simulation can be carried over to the single-column simulation. I encourage the authors to discuss this link in depth, which can be a highlight of this study. Otherwise, I don’t see the point of including a very simplified simulation of the single-column model.

This comment is likely based on the incorrect assumption that the box model simulations were a kind of direct-numerical simulation. The box model simulations does not involve any notion of fluid flow or motion of any kind, the only considered transport is that in size-spectral space. The single-column simulations add the spatial dimension, what was explicitly requested in earlier reviews. All conclusions from the box model runs (with just one spectral dimension) carry over to multi-dimensional cases including the single-column case of spatio-spectral (2D) transport.

46. P15, L15: This study focuses on...

Changed.

Thank you.