Reply to Editor Decision and the two included Reviewer Comments

The Editors Decisions and the reviewers' comments are repeated in italics. Our response is added in bold font and green colour.

Dear Andreas Bier and co-authors,

I am pleased to let you know that. based on the two reviews of the revised manuscript, your manuscript has now been accepted for publication in ACP after minor revsions (review by editor).

Both referees have final remarks to the paper (listed below) which I would ask you to consider and answer before uploading the final manuscript.

Kind regards, Martina Krämer (as CP Senior Editor)

Dear Martina Krämer,

many thanks for your positive evaluation of our manuscript revision. In the following we reply to the few reviewer comments. In addition to the modifications based on our replies, we have corrected the units in Eq. (4) of the manuscript.

Referee #1:
With their addition of some clarifications, caveats, and promises for improvements in future work, the authors have in this revised version adequately addressed the concerns listed in my review of the original manuscript, at least sufficiently for its role as a ``model development'' paper. With regards to the author's replies to my prior comments I have three further suggestions, the first for the present manuscript, the others directed more toward their future work:

(R1) In their response to my prior comments the authors provided a definition of the plume radius r_p appearing in the paper as ``the distance of the most remote trajectory from the plume centre at a given plume age'', but (unless I missed it somewhere) a definition has not been included in the revised manuscript itself. For completeness one really should be.

You are right. We have included that definition of *r_p* at the beginning of Section 3.1

(R2) The authors state that they have diffused the expected sharp gradient at the plume edge in the initial conditions to the smoothed profile shown in fig.1 in order to avoid numerical instabilities in their model. The unphysical effects of this are of lesser concern for box model applications as in the present manuscript, but will be more important in the full LES mode that the authors are aiming toward. Accordingly I strongly encourage the authors to put in some work on their numerics to avoid this in their future efforts. My answer, by the way, to the query in their comments: ``We wonder if you do not have to include such precautionary measures in your model...'', is a firm ``no''.

The trajectory data stem from the FLUDILES code. The ice microphysics code LCM, which we extended to cover contrail formation in the present study, is however coupled to the LES code EULAG. The numerical solution technique for advective transport differs between those two codes We will pay attention to this aspect within the EULAG-LCM set-up.

(R3) With regards to the question of binned versus particle-based microphysics and the resolution requirements of each: I did not state a belief in my original review that binned methods were in general superior to particle-based ones, as the authors seem to have inferred; each have their own

strengths and weaknesses. Rather I was suggesting that with the bin choices made in Lew20 and the choice of SIPs made in the present work that the former likely resolves ice and droplet spectra more faithfully. One useful set of tests I have performed in trying to determine resolution requirements for the microphysics in my own model (in addition to standard sensitivity tests) is to compare the results of different choices with exact analytic solutions where possible. In Lewellen 2012 (``Analytic solutions for evolving size distributions of spherical crystals or droplets undergoing diffusional growth in different regimes'', DOI: 10.1175/JAS-D-11-029.1), exact analytic solutions are derived that are of direct relevance to contrails. Appendix B of that paper illustrates the numerical requirements for binned microphysics schemes to match various aspects of the exact solutions at different levels of accuracy. The same exercise could be performed for particle based methods. I strongly encourage the authors to explore such tests for their planned LES work.

Even though we believe that our convergence tests (varying the number of simulation particles) are sufficient, comparison to the analytical solution of your specific test case is indeed a nice benchmark case and can be implemented to verify several components of the LCM box model.

However, we want to mention that particle-based methods often contain a probabilistic component in multi-dimensional set-ups. This implies that relatively few simulation particles in every grid box can suffice for a reliable prediction of total quantities. Only if one is interested in local quantities, (e.g., deriving a PDF of number concentration) the requirements on SIP numbers are higher. For a deeper understanding of those aspects, we refer to Unterstrasser & Sölch (2014), Unterstrasser et al (2017) and Unterstrasser et al (2020).

Referee #2:

The authors have responded to the reviewer comments in great detail and the paper is improved as a result.

I have only one further suggestion, which is to include a discussion (in Conclusions) on experimental data/evidence that would improve the accuracy of model outputs and/or allow the model to be applied more widely. For example, are there chemical and physical properties of soot particles that should be better characterised, experimental characterisation of plume dilution, meteorological observations, properties of aircraft and their engines that are not publicly disclosed. This could certainly be the topic of another paper but here I suggest that a short discussion is included to help motivate/inform/influence experimental research. After all, the authors have an insight into these important properties/parameters that would be extremely valuable to share.

Thank you for your positive feedback. Regarding your suggestion we have added following lines at the end of the Conclusions:

"**To improve the accuracy of model outputs and to enable a better evaluation with in-situ campaign data, contrail formation experiments should include in addition to total number concentrations measurements of exhaust and ice particle size distributions. Due to the large spatial heterogeneity and fast change of thermodynamic and microphysical quantities, a precise determination of contrail age and sampling position in the plume is crucial. High resolution measurements of water vapour can help to characterise the growth and sublimation of ice crystals. A thorough discussion of benefits and limitations of different measurement strategies are valuable to understand how a quantitative comparison of modelled and measured data should be performed."**

References

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