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Comment on acp-2021-361

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Referee comment on "Box model trajectory studies of contrail formation using a particle-based cloud microphysics scheme" by Andreas Bier et al., Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2021-361-RC1, 2021

This is primarily a ``model development'' paper, extending an existing microphysical cloud model (LCM) to allow simulation of contrail formation. This is implemented at a box-model level as a step to future incorporation within a 3D LES. Most of the text is devoted to describing the necessary additions to the microphysics and to testing the resulting model with a small parametric box-model study. Neither covers particularly new ground in the literature, the added microphysics being pieces already utilized for this purpose by prior researchers, and the box-model parametric study results being consistent with, and much less extensive than, prior studies using box models (e.g., Karcher and Yu 2009) over even full LES (Lewellen 2020). Nonetheless, given the complexity of such simulation codes, the successful comparison presented provides a useful crosscheck on the prior work, and the generally clear documentation will provide a useful reference as the authors proceed with future model development and contrail studies. The most novel part of the present work are the simulations run in the ``ensemble'' mode, in which box-model simulations using dilution histories from a large representative sampling of Lagrangian trajectories from a 3D LES are averaged over. The ultimate utility of this method is, however, highly questionable (for reasons discussed below) and so the main benefit here may be as a cautionary tale. Perhaps not surprisingly, my review here is weighted more heavily to the comparisons in the text with my own work (Lewellen (2020), denoted Lew20 hereafter).

Main points:

(1) The paper makes clear that the eventual goal is to incorporate the modified LCM within a particular LES (EULAG) for 3D contrail formation studies. But it doesn't motivate why the use of this computationally much more expensive approach may be required, or give any hints of the hurdles to be overcome for using EULAG for this purpose. A brief statement or referencing for both would seem useful to the reader. Lew20 provides relevant content on both counts: the simulations there illustrate that in some broad regions of the physical parameter space the box model results differ substantially from the LES ones, and several of the difficulties involved in modifying an LES (even one already capable of simulating aging contrails) for the distinct environment required to study initial contrail formation are described.

(2) I think that variable-density/compressibility effects are not being properly taken into account in the plume dilution equations in sections 2.3.1 and 2.3.2 where it is assumed that temperature dilutes like a passive tracer. Masses are conserved in the exhaust plume, but density and temperature are (by the ideal gas law and the near constancy of pressure in a free jet) inversely related. For temperature to be conserved as a passive tracer to good approximation then requires the temperature differences encountered to be small relative to the absolute temperature. While this is a reasonable approximation in most atmospheric models, it does not generally hold in the hot jet exhaust plume until sufficient dilution takes place. The nature and limits of the approximation being made here deserves at least a mention in the text. This deviation of T from a passive tracer is in addition to that from the conversion of jet kinetic energy to thermal energy (noted in line 270). Treating T as evolving like a passive tracer with no corrections (as assumed) will lead to the largest inaccuracies here for the ``ensemble'' cases because contrail formation commences earlier there and because that relation has been used to define the ensemble itself via equation (17).

(3) A sizable portion of the paper is spent on the ``ensemble'' trajectory approach. Even while using a large number of trajectories from an LES run, thus providing some detailed spatial information, this approach leaves out a crucial piece of physics: the microphysics along each of the trajectories is computed independently of what is happening on the others. In reality all these various parcels are mixing with each other so that moisture condensed on aerosol in one parcel will not be available later to condense on aerosol in other parcels it mixes with. It is this competition between different parcels that Lew20 concluded was responsible for box-model results sometimes greatly over-predicting ice number relative to LES results. The ``ensemble'' mode gets this entirely wrong, predicting a higher ice number relative to the ``average'' box model results. These shortcomings are noted eventually in the main body of the paper (pg. 24), but only after promising statements are made about the method earlier (e.g., line 88), and they are not reflected in the abstract or conclusions. This likely gives a misleading impression of the potential utility of the method. I would suggest remedying this omission. Indeed, the illustration of this cautionary tale could be the most useful new result in the present paper, given that others may be tempted to use this approach in different applications (or have already). It would also be worth explaining (if the authors know) why the

``ensemble'' freezing fraction always lies above that for the ``average'' box model when they differ. I suspect this may involve the specific averaging procedures employed, which are not specified in detail in the text and seem to rely on treating temperature as a passive tracer (c.f. lines 286-287).

(4) Some of the statements in comparison to Lew20 are perhaps misleading. First it is stated (lines 20, 614) that the results of the present model and Lew20 on a comparison case are in excellent agreement. This is true when comparing to the box model results of Lew20 (which does provide a useful check on the microphysics) but not with the LES simulation results from Lew20 of the same case, which differ significantly (i.e., compared to the best results of Lew20 on this case the agreement is in fact not so good). Also, referring to this as a cross-validation (line 20) is too strong: since the present work uses many of the same parameterizations in the microphysics as Lew20, it would be possible to have excellent agreement between the two models even if one of these parameterizations were to turn out to be physically poor.

Later, it is suggested (e.g., lines 64-67, 78-79) that the scheme of representation of particle sizes in the present model will improve upon that utilized in Lew20, but that is not at all clear. Although Lew20's LES model itself will allow for more complicated soot spectra (at increased numerical cost), Lew20 presented results only for mono-disperse and bi-disperse soot spectra. This was sufficient to show through examples that the final results were not very sensitive to the details of this size initialization, justifying the simplification, and directly contradicting the supposition here in line 65-67 that it might lead to too narrow ice spectra. Lew20 found in practice that having well-resolved droplet and ice size-spectra was the much more critical requirement to properly representing competition between different sized aerosol populations in the exhaust plume. In that regard the binned microphysics representation of Lew20 would seem to have the advantage over the particle-based description used here. Given the modest number of SIPs utilized here to represent the entire spectral shape (c.f., lines 143-146), the binned scheme with a healthy number of bins (as in Lew20) can more faithfully represent size spectra, particularly in the tails of the distributions that can play an out-sized role.

(5) The explanation of the differences between the results for the dilution histories from FLUDILES and Lew20 (lines 509 and following and section 5) could be sharpened significantly by making use of additional results given in Lew20. The authors attribute the slower plume dilution in the FLUDILES case to using temperature to deduce the dilution history without properly accounting for the conversion of jet kinetic energy to heat. This is a likely contributing factor (as perhaps is the issue in item (2) above), but a large part of the dilution rate difference between the FLUDILES and the baseline Lew20 case seems to be a perfectly physical one: the former simulation is apparently for a larger engine than the latter (initial plume radius of 0.5 m as stated in line 255 for the former, versus an initial plume core radius of 0.3 m in the Lew20 base case). Lew20 includes an analysis of

the effects of increasing engine size, including the resulting increase in dilution time scale. Further increasing the dilution time scale is the choice in FLUDILES of an excessively smeared initial profile at the plume edge (line 264-265 and fig. 1a). Finally, Lew20 included a large parametric study varying the engine size (and hence dilution rate) and explained the differences in ice numbers that resulted. The variations with dilution-rate seen here in fig.7 all seem to conform (at least qualitatively) with those prior results.

(6) While the simulation cases are generally well described, some of the specifications are missing, vague, or departing from physical expectations. What engines are assumed? Is the bypass treated and if so, how? The radial gradient of the plume at the engine exit (c.f., fig. 1a) seems unphysically spread out. Line 265 implies this is for numerical reasons (why?). And given this gradient, how is r_p (line 343) actually evaluated? Lines 297-298 state that the fuel consumption has been adjusted, but the description why is vague and the value of m_f is never actually given. Under normal cruise conditions engine parameters (and hence properties of the exhaust jet) will generally shift some with ambient temperature. Are these effects at all included in the T_a varying cases considered. If not, that should be noted. Some of these questions may be addressed in Vancassel et al. (2014), but the present paper should be self-contained on the basic specifications and levels of approximations employed.

(7) The physical parameter space of relevance to contrails is very large (ambient conditions, aircraft-dependent conditions, aerosol content, etc.), only a tiny select fraction of which is sampled in the simulations here. Accordingly, some of the statements of results in the paper are stated too strongly or too broadly and need added qualifications so as not to mislead some readers: they may be true for the specific simulations conducted, but that doesn't mean they hold across the full parameter space (and in some cases definitely do not). Examples include the statements in lines 16-17, 456-457, 467-468, 476-477, and 600-602.

(8) The authors are likely overstating the importance of the ``deactivation phenomenon'' they identify in lines 393-401 in explaining reductions in freezing fraction. While such reductions are almost certainly due to competition for available moisture between different aerosol populations (as discussed in Lew20), ``deactivation'' is only one such mechanism involved. The alternate mechanism of competition between aerosol for moisture preventing some aerosol from ever activating (rather than activating and then deactivating) is generally more responsible for reductions in ice number (judging from the larger parametric study of Lew20).

Minor points:

(9) line 40: Contrary to what is implied in the statement, large enough supersaturation to form ice starting from ultrafine aerosol can be produced in jet exhausts fairly easily (as is shown in Lew20).

(10) lines 132-134: The statement is misleading. Just as one can include a soot spectrum without necessarily modeling its formation, one can usefully include ultrafine aerosol without modeling its formation from ion clusters (as done, e.g., in Lew20).

(11) Some of the figure captions need additions to make the figures more understandable on their own. For example some of the description following line 340 should be moved from the text to the figure caption. And the red and blue lines should be identified in the fig.4 caption.

(12) The wording in lines 351 and 354 is somewhat misleading. While RH_liq increases with time and radius within the bounds of fig 1 it does not do so indefinitely: for large enough radius and time it decreases.

(13) line 446-447 is misleading. Since the ambient is supersaturated in the case illustrated in fig.4, conditions don't drop back to ice saturation and the crystal size continues to grow (albeit more slowly).

(14) In line 530, differences due to different turbulence realizations in the Lew20 LES results are described as an ``irreducible'' uncertainty. This is not strictly true: one could average over an ensemble of such LES results to reduce this uncertainty (at additional numerical cost).

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