Review of

"Simulation of a contrail formation and early life cycle for a realistic airliner geometry"

By Bouhafid and Bonne

Summary

This study present simulations of early contrails with an advanced CFD method. The paper is well-formulated and the results are clearly presented. Basically a few simulations with an high-fidelity dynamical approach are analysed and the impact on the type of wake vortex and exhaust plume initialization and on stratification are discussed.

General comments

The comparison between the RANS-based and analytical wake vortex initialization is in general well-described. I appreciate the efforts with the 4LO initialization that tries to mimic the RANS initialization by simpler means (future applications might use the 4LO initialization and do not require a-priori RANS simulations of the initial vortex roll-up phase).

We identified several major issues (mostly in the study design and analysis of the simulation data) that should be addressed in a revised version

1. The analysis of the extinction and optical depth of young contrail may be misleading and misinterpreted by readers.
   a. The contribution of the first few minutes of the full contrail lifecycle to the time-integrated radiative forcing (or extinction) is usually not substantial. A relatively larger extinction in the beginning does not imply a larger radiative impact at later times and in total.
   b. Simulations in Unterstrasser & Gierens (2010b) and Lewellen (2014) show that the total number of ice crystals is the most crucial quantity of young contrails that determines the further fate. The early ice crystal mass (and also optical depth and integrated extinction) does not significantly affect the long-term behaviour of the contrail-cirrus transition. Hence, an evaluation of total ice crystal number would be more insightful.
   c. Moreover, I strongly suggest to not use the term "radiative forcing of young contrails".
   First of all, radiative forcing is defined as a radiative imbalance typically evaluated at the top of the atmosphere and this is not what is evaluated in your study. You should make clearer, how to interpret the extinction quantity that you analysed.
   d. In line 515, the conclusion states, e.g., "RANS initialization produced a more turbulent contrail with ... increased radiative impact". I think this formulation is too strong. Similar formulations appear in other locations as well.
2. How robust are the evaluations of Δz and Δy? In Eulerian models, contrails typically do not feature very strong gradients at the boundaries and fade out. Hence, the values you determined may depend on thresholds with which you define a contrail. I believe it would help readers to also show vertical and transvers profiles of ice crystal number

and mass. This would allow for a more quantitative comparison compared to Figs. 7, 8 and 12 and also makes clearer how robust the evaluations of Δz and Δy are.

3. How is the boundary of the contrail defined? Why do you choose to apply a weighting by number? Why at all and why not by ice mass e.g.? No spatial distributions of ice crystal number concentration are displayed. Nor the time evolution of total ice crystal number is shown. Hence, it is not transparent what effects the weighting in the averaging procedure does introduce.
4. Your analysis focuses on intensive mean quantities, which depend on the contrail-cross-section of the contrail. It would be interesting to also see integrated quantities like the total ice crystal number and mass (which do not depend on the definition of the contrail boundary).
5. Your interpretation of the simulation results focuses on the differences in the dynamical setup (RANS versus 2LO and 4LO). It is not much discussed that in addition the exhaust plumes are initialized in a different way. Currently you simply assume that observed differences in the simulation results are due to the different wake vortex initialization, but this is not really proven. It may help to perform another type simulation where the RANS with the idealised exhaust plume or the LO wake vortices are combined with the RANS exhaust plume. This way you could answer, which of the two aspects is more crucial.
6. Why do your simulations run up to t= 200s? Previous contrail vortex phase simulations considered a longer time period (5 minutes or longer). Have the vortices decayed after that time? Both N_b values represent strongly to extremely stable conditions. Air masses that move downwards will rise when the vortices get weaker. Is this process already completed at t=200s? It would be interesting to see whether vertical profiles change more slowly after the vortices break up and buoyancy-driven air motions cease. Is this already the case after 200s?
   The background of the question is that Fig.8 shows a strong difference after 200s between 'RANS' and '2LO'. It is not clear if this discrepancy is just a transient phenomenon and whether the difference between the two simulations is long-lasting (as the vertical distribution does not change much beyond t=200s).
7. Line 155: What do you mean with heterogeneous nucleation? The scientific consensus is that contrail formation occurs on condensation nuclei via heterogeneous droplet nucleation, with subsequent homogeneous freezing. Referring to heterogeneous nucleation may imply that soot particles act directly as ice nuclei (IN). In Equation (9), it appears that soot particles are assumed to become ice crystals immediately upon activation. Why is the liquid phase and the freezing process not explicitly represented in your model?
   Another manuscript in review for ACP by Ponsonby et al. (https://doi.org/10.5194/egusphere-2025-1717) states: "To that end, several LES models prescribe water saturation as the critical condition for contrail ice formation (Paoli et al., 2013; Picot et al., 2015) or heterogeneous ice nucleation as the primary formation pathway (Khou et al., 2017, 2015), both of which have been rejected by in-situ observations (Kärcher et al., 2015). More representative microphysical treatment can be achieved using 0D box- and parcel model simulations (Bier et al., 2022; Rojo et al., 2015; Yu et al., 2024). Here, the dilution of a parcel of exhaust air is simulated and microphysical phase transitions such as particle activation and homogeneous ice nucleation are tracked. While these models are unable to incorporate feedback between different plume parcels, which may otherwise lead to a diversity of particle history

(Lewellen, 2020), they are configured for sophisticated treatment of complex ice microphysics, which is critical for describing contrail properties (Yu et al., 2024)."

Specific comments

- Line 2: The accumulated CO_2 emissions by aviation
- Line 12: Make clear that this statement holds only for young contrails. Emphasize that further research for long-lived contrails is needed.
- Line 16: replace nucleation by condensation
- Line 44: The ice crystals do not heat up adiabatically. The surrounding air does so with implication on the relative humidity and ice crystal growth.
- Line 50: Do those vortex rings always form?
- Line 52: I would prefer to reformulate to something like "Contrail evolution is driven *or governed* by physical *processes* (not by conditions) which are affected by *(conditions like)* wind shear, stratification etc.
- Line 55: Lewellen (2014) is also a great source of contrail-cirrus analyses.
- Line 117: to form ice crystals, condensation is not enough, you should explicitly mention also the freezing process.
- Line 126-127: already stated in line 115
- Inclusion of Eqs. (7) -(9) into the text would facilitate reading.
- Eqs. 2, 3 and 6 do not convey a lot of information. With which rates do those conversions occur? Would it be more informative to write the equations for the mass fractions of all or selected quantities?
- Section 3.2 does not explicitly mention how water vapour is initialized. The sentence in line 281 may imply that absolute water vapour mixing ratio is held constant with altitude. Most other studies of the contrail vortex phase kept the relative humidity constant. Could you plot RHi(z) to see how much this quantity changes with altitude?
- Fig. 9: the contrail height and width evolution of the RANS case with N_b=0.03 s_{-1} looks a bit strange in the sense, that at t=4.5 the height suddenly stops to increase (which might be linked to vortex break up) and width increases. What process leads to such a large change in the width increase?
- Section 4.1. It would be interesting to also see the time evolution of total ice crystal number I and mass M and possibly also of the ratio Nice/Ns. M_{ice} and N_{ice} are more straightforward to analyse and interpret than the derived mean radius ~ $(M_{ice}/N_{ice})^{1/3}$.
  Computing the mean radius via M_{ice} and N_{ice} is probably better than evaluating r_p in each grid cell and do a number-weighted average. How much do the computed values differ between the two formulas?
  The formula in line 325 might be interpreted in a way that r_p depends only on IWC. I would prefer to include N_{ice} in the formula.
- Lin330: If all soot particles are activated and more ice crystals are present, then they should be smaller not larger if ice mass is similar.
- Line 361: It is not clear, if the scaling of time is applied in the model or only in the presentation of the results. What's the advantage of using a normalized time coordinate in this study? All setups have the same t_0 and there is no benefit of normalization to make results better comparable. If you keep the normalized values, it would help the readers to add the t_0 value to the figure captions.

- Fig.7. shows soot number density which is not an actual contrail property. Wouldn't it be more logical to show contrail ice crystal number or mass concentration?
- Line 374: this sounds like a general statement about contrail formation in strongly stable conditions. But I guess it only relates to your choice of water vapour initialization. Do you mean the actual formation process or the time evolution over 200s?
- Fig.11: Trends are very similar. Do you expect a long-lasting impact?
- Eq. 19: I believe in the contrail community, the quantity defined in Eq. 19 was first introduced in Unterstrasser & Gierens (2010a) and named total extinction.
- Line 439: Yes, that is the important point. I would appreciate to see this statement also in the abstract.
- Line 504: The statement is too strong for reasons stated above.

Technical corrections

- Figure 1: replace M_{infty} by U_{infty}
- Line 21: estimation of effective radiative ERF of contrails and other forcing agents.
- Line 24: Is controversial the correct word here? What fact is controversial?
- Lines 103 and 195: "negelected before" does not sound like proper English
- Line 114 "water vapour H2O" = "gas-phase H20"? Similary, ice-phase $H20_s$
- Line 155: Contrail (without 's') ice
- Section 3.2 should state the time period that is simulated.
- Line 301: weighted
- Line 330: soot PARTICLES
- Figure 5 and Figure 10: soot number density is named N_s and N_p. Please be consistent.
- Figure 7: The r_p values on the colour bar should have nice values. Is a linear or logarithmic scale used?
- Line 378 Widnall
- Line 382: length scales
- Line 395: descend
- Line 395: 'contrail surface reduction': do you mean a decrease of the contrail cross-sectional area?

References

Lewellen, D. C.: Persistent contrails and contrail cirrus. Part 2: Full Lifetime Behavior, J. Atmos. Sci., 71, 4420–4438, doi:10.1175/JAS-D-13-0317.1, 2014.

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