An updated microphysical model for particle activation in contrails : the role of volatile particles

<u>Overall</u>: This paper update two different microphysical model and perform sensitivity analysis to input parameters with only one of this model, the one that seems the most realistic. Their update consist in adding a distribution to account for volatile particles in order to be able to compute contrail formation in low soot regime. Overall the model modification are well explained as well as most of the underlying hypothesis; however several informations are missing such as what is the density of the volatiles particles, the surface tension… The number of volatile particle is fixed and their appearance process is not model. This limitation is clearly mentioned. But I regret the lake of sensitivity analysis on this parameter of the model.

Major

The paragraph 4.4 is interesting. This kind of graph have already been made by https://doi.org/10.1021/acs.est.4c04340 and https://doi.org/10.21203/rs.3.rs-6559440/v1 how do your graph compare to these papers?

Line 592-595, you status that volatile mode characteristics on POM and FSC has not been talked at curise altitude. However Rojo et al 2015 clearly include POM in their volatile and they perform a sensitivity analysis to FSC and POM emission index on contrail formation.

In line 577-581 you underline the impossibility of dvPM being found by equation 22 but you tell in line 459 that you use it to estimate this diameter. Therefor I m a bit lost. Do you use this formula or not? If yes, what is the error made by this choice?

I will assume in this comment that you use the formula 22 to choose the initial diameter of the volatile particles. In order to find it, you need to define the density of the volatile particles. However, you give no indication of its value. Please provide this information. The same remark can be made for the surface tension, what value do you use?

You perform a sensitivity analysis on the volatile particle emission index by doing 0 or 1e17. Since this is a major hypothesis of your work, I suggest a more detailed sensitivity analysis such as EI=1.e16-18 for example.

In the acknowledgement you mention Christiane Voigt for “model comparison with in situ measurement”. If you have access to experimental data, why don’t you show some experimental validation of your model?

For what I understand of the model, every volatile particles are a mixture of organics and sulfuric acid. Considering that the organics are mainly insoluble species and sulfuric acid is soluble, is there no possibilities to have in fact two different kind of particles one of pure sulfuric acid and one of pure organics?

Minor:

Line 45-48: You give an experimental definition of volatile particles which is right, however the reader may be confuse if these particles exist or not at the exit of the engine. I suggest adding a sentence, which says that considering the exit temperature of the engine, the volatile particles forms during the cooling of the plume.

Line 50: you give a value for the apparent emission index of volatile particles of 1E17 kg-1. In a recent paper (still a pre-print) https://doi.org/10.21203/rs.3.rs-6559440/v1 they show inflight measurement. The total particle number is limited between 5E14 and 5E15, depending of the flight condition and fuel used. Since this is an order of magnitude lower, it would be great to add more references from the literature.

Line 75-80: I suggest you to read https://doi.org/10.1080/02786826.2024.2395940 and https://doi.org/10.1016/j.jaerosci.2025.106612 which introduce in complex CFD a microphysical model which seems close to the one from Wong 2014 model.

Line 226-227: “However, as outline in SIS3, this criterion cannot be reconciled with minimum requirement for particle activation” is a bit too negative since particles may be already big enough to be activated has shown by line 245-251. I suggest to restrict this statement for small particles.

Line 270: you neglect the uptake of water of the atmosphere while you take into account the uptake of ambient particle. I agree that at first it is negligible but at the end it will probably influence the size of the ice crystals. Considering the low cost of such modification I don’t really understand why have you done this choice.

In equation 16 you neglect the variation of temperature due to freezing and condensation whereas in the Pyrcel website it is included. Can’t it also be included in K15? Moreover in the Pyrcel description in lines 407-412 you replace the gravity term by the one given in this equation, do you keep the latent heats term?

In line 450-453 you distinguish between oil organics and gaseous emission. In line 461 I have the impression that you treat them as the same species. Are they treated the same way?

You conclude 4.3 by telling that Pyrcel is better than K15 but in line 554 you tell that you make the sensitivity analysis with K15. I guess you have use Pyrcel but it is just a typo.

In line 645 you say that the K15 model could be incorporated in global contrail simulations, however considering the comparison with Pyrcel, I wonder why K15 and not Pyrcel?

In Supplementary material S1, figure S1: please recall the k value used in order to simplify the reading.

Limitation given in line 351-354 has to be emphasis in the introduction since it is an important one.

In line 54 of the supplementary material, you give the probability to transform into ice. Then in line 56 you say that the particle freeze when the probability is one. However, the line 54 formula shows that this probability is never equal to one. Then you have to choose a threshold. You have to give the information to the reader.