Response to referees: Physical characteristics of frozen hydrometeors inferred with parameter estimation, Alan J. Geer

The reviewers' comments are included in black. The responses I gave in the discussion are interleaved in blue. A description of the final changes to the manuscript is given in red, with line numbers referencing the DIFF version of the manuscript.

Anonymous referee #1

This study develops a physically consistent means of combining NWP model simulations with a simplified radiative transfer (RT) model to estimate both the micro- and macrophysical properties of frozen atmospheric particles with the ultimate goal of improving physical constraints in operational forecasts of clouds and precipitation. I have felt for some time that such an approach would be useful in data assimilation where these physical parameters would be part of the state vector solution. However, the author has done a good job of highlighting and explaining some of the significant challenges of using parameter estimation within a DA system.

One of my main concerns with using coarse-resolution model simulations and simplified RT models is that the parameter estimation will simply reflect the NWP model biases (such as caused by sub-grid-scale parameterizations) and uncertainties in the RT model. In addition, the parameters will require continual updating based on changes to the model parameterizations and complexity of the RT model. However, the author has fully addressed these concerns in section 6.

An important conclusion of this study is the importance of utilizing a wide range of microwave frequencies to constrain the strong frequency dependence of single-scattering properties, which are sensitive to the particle size distribution, mass-size relationship, and particle density and shape. However, the author makes clear that "the particle habit itself is not being precisely identified, but rather the full 'hydrometeor model' which is controlled by the choice of particle habit in the current framework but includes also an assumed mass-size relation." This is an important clarification because there is often a misconception that particle habit is solely responsible for reducing biases in forward RT calculations at high microwave frequencies when compared to observations.

Finally, this study not only discusses the limitations of the method but also offers a way for improvement and describes how it builds on earlier work.

My only complaint is that the paper is rather long. The concern is that readers may be less inclined to read the paper in its entirety and may overlook some of the nuances and important results of the study.

In summary, the author has done an excellent job of articulating a complex problem in simple, understandable terms and in demonstrating the general applicability of the method to other NWP models and RT models.

Thank you for your review and for your comments. The issue of length is a good point and I will try to make any future work shorter. However it would be hard to cut anything out of the current manuscript at this stage; many aspects are already covered with less detail than would be ideal.

Minor points:

Line 53: Typo: "There is also a need …"

Line 230-231: Actually, the South Dakota School of Mines and Technology T-28 storm-penetrating aircraft has, for decades, flown through convective cores to take in situ measurements of hail and graupel (e.g., Detwiler et al., 2012, Bull. American Meteorol. Soc.; Field et al., 2019, J. Appl. Meteorol. Climatol., 58, 231-245).

I am very grateful for the pointer to the historic work with the T-28 storm-penetrating aircraft. The recent work using this dataset to describe hail PSDs (reaching up to at least 5 cm, Field et al., 2019) would clearly be a good future alternative for the PSD representing the "convective snow" category, rather than repurposing PSDs intended for other hydrometeor types, as done in the current work. In the revised manuscript I will adapt the relevant discussion on lines 228 - 235 to reflect this, and to acknowledge that some direct observations inside convective cores do exist; also perhaps mentioning the recent balloon-borne measurements of Waugh et al. (2020) if space permits. I will also try to fit this point into the discussion or conclusion of the revised manuscript, if at all possible.

The relevant paragraph (lines 237-250) has been much changed to be more precise about hail sizes and to include discussion of the T-28 aircraft. The suggestion of using the new hail PSD is added to the discussion on lines 610-611. Line 710 is changed to reflect the work of the T-28. Line 766 - 767 in the conclusion repeats the suggestion about the hail PSD.

Line 309: "approx." should be spelled out.

Fixed on line 322

Line 377: Typo: "shape of the cost function is very different"

Line 402

Line 582: Typo: "If they had done that …"

Line 634

Line 624: Typo: "it is important to …"

LIne 676

Line 635: Typo: "a little bit like …"

Line 688

Line 723: Typo: "in the future …"

Line 781

Anonymous referee #2

Paper Summary:

Our understanding of ice clouds and ice particle characteristics globally, and especially in deep convection, is sorely lacking. The author aims to address aspects of this problem via perturbation of six parameters relevant to frozen hydrometeors in the ECMWF assimilation system, with the goal of simultaneously adjusting parameters in such a way that simulated microwave radiances agree with observed microwave radiances from F17 SSMIS (for 13 channels, extending from 19 – 183 GHz) over a 13 – 22 June 2019 test period. An output of this study is improved frozen hydrometeor assumptions to be used in version 13 of RTTOV-SCATT.

Major Issue(s) and Comments:

One major issue I had was the lack of discussion on mixed phase microphysical processes and presence of super-cooled liquid in the "frozen" tops of convective cores. A neglect of this implies that ice particle parameter settings will likely have unphysical settings or values due to scattering signatures in convective regions having to be matched by varying only ice parameter degrees of freedom. If variations in liquid (at the expense of ice) were allowed, simulated microwave Tb signatures would be substantially different since liquid would cause emission instead of scattering, thus impacting the choice of ice parameter settings (and potentially allowing graupel to occur much more frequently). We can comfortably neglect liquid at cold icy temperatures in the weak ascent regions of stratiform clouds, but since convective ice is a particular focus of this paper (which is certainly welcomed given the lack of convective ice papers), then at the least, some discussion of the role of liquid at cold temperatures in convection must be discussed. Clearly some of the results for perturbing convective-ice related parameters signify a compensation for lack of liquid allowed in convection, and thus, parameter values decidedly returned are also likely not realistic due to this neglect. The number of studies documenting the prevalence of liquid down to minus 37.5 deg C in convection are numerous and increasing (e.g., in general, independent of aerosol effects or discussion: Kumjian et al. (2012; JAS); Dolan et al. (2013, JAMC); Xu and Zipser (2015, JGR); van Lier-Walqui et al. (2016, MWR); Fuchs et al. (2018, JGR), and within the context of aerosols: Rosenfeld and Woodley (2000; Nature); Fan et al. (2018; Science)). In short, importantly, liquid/graupel/hail is a microphysical phenomenon common in the cold tops of convection, further evidenced by the commonality of lighting in convection globally. I would not be terribly surprised if the lack of choices regarding choosing graupel/hail in this study (and others) relate to our underestimation of liquid in the upper reaches of convection. At the very least, this should be given distinct discussion within the context of the parameter settings determined.

Thank you for your review and for your comments. The main issue of supercooled liquid water (SLW) in deep convection is an important point and I appreciate your introduction to the literature on this. As suggested, I will add some discussion, likely in the conclusion of the revised manuscript. The basic point is well taken that the existence of lightning in deep convection, and the rimed particles that generate it, requires significant mass of SLW above the freezing level, likely both raindrops and cloud liquid (e.g. Kumjian et al., 2012; Fuchs et al., 2018). The IFS model broadly does not represent SLW within convection. This issue has already come up, for example in the need to detrain a higher proportion of SLW into stratiform cloud in order to correctly represent shallow convection in cold air outbreaks (Forbes et al., 2016). It would be possible to use the parameter estimation framework to explore alternative partitioning between ice and liquid, as you propose in minor comment 4, however I would like to leave such a substantial additional piece of work to a future study.

My guess is that properly representing SLW will make the representation of strong scattering brightness temperature depressions in deep convection even harder. As illustrated in Geer et al. (2021), above 100 GHz, the bulk optical properties of rain provide a single scattering albedo (SSA) of around 0.5, as compared to around 0.95 from completely frozen particles. This means that liquid droplets above the freezing level will likely provide strong absorption and emission, so that they will be able to increase the brightness temperature of the cloud towards the physical temperature (e.g. 200K) and away from the scattering-dominated brightness temperature of the cloud (e.g. 100K or less). These mechanisms are described in a little more detail in Geer et al. (2021). I will try to make this point compactly in the conclusion of the revised paper.

The issue of convective supercooled rain is now covered in the discussion on lines 604 - 610, and mentioned in the conclusion on lines 766 - 767.

Minor Issue(s) and Comments:

Is noise in observed microwave radiances considered at any point?

Noise in observed radiances is not considered at any point in this work. Currently, noise is irrelevant to the modelling of cloud and precipitation-affected radiances, where the modelling errors may be at least 10 K in brightness temperature, and the instrument noise may be around 0.5 K (e.g. MHS, https://space.oscar.wmo.int/instruments/view/mhs). This point is explored in more detail in Geer and Bauer (2010); I will see if it is possible to mention this in the description of the cost function in section 4.2 of the revised manuscript; certainly there is no need to represent the true observation error explicitly in the parameter estimation.

Discussion added on lines 381-383.

When it is said that mixing ratios are halved/doubled, does this mean for all altitudes equally, from above the melting level to cloud top?

On the mixing ratio adjustment, yes this is done simultaneously at all altitudes. This point will be clarified in the revised manuscript.

This was clarified on lines lines 231-232

The 20K discrepancies in Fig. 4 are sort of glossed over mostly due to occurrence frequencies, but I suspect they are the convective regions (convection by frequency of occurrence is of course small relative to ice cloud in general, so this seems plausible). Would a map of the large discrepancies be correlated with deep convection patterns or no?

On the validity of the assumption of linearly additive perturbations, yes, the larger errors of 20 K are predominantly in convective areas over land (as judged by plotting them on a map, for example). These are the locations where the revision to the cloud overlap has had most effect on the brightness temperatures, seen also in Fig. 8 in the submitted manuscript. Another way to quantify these errors is as a fractional error: by this measure, the assumption of linear additive perturbations underestimates the larger TB (>10 K) increases by typically around 30%. Also, on revisiting these results, I discovered one mistake in the text: the overall standard deviation of the differences is 0.96 K, not 0.2 K as stated. These numbers and additional discussion will be added to the revised manuscript. Another way to judge the validity of the assumption is to compare maps of the mean and skewness measures that are used in the cost function; these are nearly identical to a visual inspection (based on figures equivalent to Figure 7 in the submitted manuscript). The assumption is not perfect, but it was vital as a way of making this work practically achievable. Based on this discussion, I would also like to add a line or two to the conclusion to say that future work should include further testing of the validity of this assumption; it should not be just relied upon by future investigators.

The paragraph on line 330 to 340 is much altered to more precisely describe the errors shown in Figure 4, to describe the link between the large errors and convection, to also mention the surprisingly good mapped statistics obtained from this assumption, but to finish on a note of caution on the general validity of the linear assumption. Line 682 is corrected to use the percentage error (not the Kelvin error, previously incorrectly described as %). Line 686 - 690 in the discussion makes it clearer that the validity of the linear assumption is limited and it will always need further checking in any new applications. Lines 779 - 781 make the same point in the conclusion.

Related to the issue of large fractions of liquid in convective cores, if something so simple as an effective cloud fraction (C) can be used as a parameter, could a simple factor that governs the amount of convective condensate partitioned into ice vs liquid (with the latter describe bed using a M-P DSD for simplicity) be incorporated quite easily as well? Or, even, couldn't the temperature for freezing in convection simply be modified to vary from 0 deg C to approx.. minus 37 deg C?

Yes, as mentioned above, it would be possible to explore alternative partitioning of the ice and liquid in convection. Some discussion around the importance of supercooled liquid water in convection will be added, probably in the conclusion of the revised manuscript.

These ideas were a little too detailed to include in the eventual discussion on lines 604 - 610, but they are clearly good ideas to try for the future.

Abstract, first sentence, Line 2: I recommend replacing 'models or satellite observations' with 'model grid boxes or satellite observation fields-of-view'.

This is a good suggestion to be more precise about the model resolution and the satellite field of view in the first sentence of the abstract; I will include it in the abstract of my revised submission (word limit permitting).

This is changed on line 2

Anonymous referee #3

This article describes a major upgrade and its physical justification of the frozen hydrometeor parameters in the radiative transfer model of RTTOV relevant to microwave and submillimeter wave spectrum. In the macro-scale, this upgrade revised a cloud overlap scheme and introduced a new "convective snow" that is analogous to the cumulus parameterization in non-cloud-resoling models. In the micro-scale, new particle size distribution and ice/snow particle shapes are introduced. In the parameter selection procedure, the cost function is configured to match the PDF between calculated and observed brightness temperatures, which is innovative. I found that the author has done a thorough examination to this parameter selection problem and worked his best in this inter-tangled web of uncertain parameters to find the best configuration for practical use. The effort is commendable. The structure of the paper is logical, and the writing is easy to follow (although a little lengthy). I recommend accept after some minor revisions. The following are my concerns.

Thank you for your review and for your comments. The point about the length of the paper, consistent with reviewer 1, is taken onboard for future work, but it would be hard to adjust the manuscript now without cutting important details.

Although the new (Final) configuration seems to be more physically sound, as a reader, I am not clear how the cost decrease from 0.932 to 0.911 translates to real improvement. I believe that Figure 5 is intended to show the impact, but neither the figure nor the explanation make me feel clearer about the impact. Therefore, I'd like to suggest: (1) improve Figure 5, so that it can show the result from the "Best" is closer to "Observations" than "Control", (2) add more explanation to argue the "Best" is better than "Control", and (3) add a PDF figure to show the PDF shifted more closer to "Observations" when "Control" is replaced by "Best". The author may also try some other ideas. The point is: how to translate the cost decrease to easy-to-understand improvements.

The point is taken that it is hard to get a sense of the improvement going from the control to the improved configurations, based on the global measures of cost. However, Figure 5 is intended to show the shape of the cost function and to illustrate the technique, whereas Figures 7 and 8 are already provided to try to illustrate the changes, such as improvements in simulating extratropical convection over land, and slightly worse fits in tropical convection over land. I will try to add the PDF of simulated and observed brightness temperatures to the revised manuscript, as suggested. However, although it shows improvement, this is not very large. The problem is that there is not a big overall improvement in fits to observations (and I hope the manuscript does not imply this). The reduction in cost from control to the "best" configuration is only from 0.925 to 0.908, as already mentioned on lines 391-392 of the submitted manuscript (note that the "final" configuration, from Table 7 is a little separate from the main part of this work so I will concentrate on the "best" configuration from Table 4, which is what Figure 5 refers to).

It is also worth restating that the achievement of the global parameter search was not so much to provide an overall improvement in fit to observations but to provide a more physically realistic underpinning for the simulations that should support future developments (e.g. the more physical cloud overlap, the use of a non-spherical particle for cloud ice for the first time, the use of ARTS database particles to support future sub-mm work).

On lines 417 - 420 the text is now even clearer to say that the reduction in cost function is small and associated with a mix of degradations and improvements. Lines 435 - 471 are extensively rewritten, making reference to the new figure 8, containing the requested PDFs. This helps do a better of job of quantifying the improvements in the "best" configuration but also showing the trade-off between tropical degradations and extratropical improvements.

The "snow mixing ratio" dimension is peculiar. As I understood it, it is rooted from the uncertainty in particles' falling speed when you convert from mass flux to water content. But still, altering mixing ratio doesn't seem to be a sound approach. Fortunately, in the "Final" configuration it is decided not to change it. I'd like to propose to eliminate this dimension in the first place.

I acknowledge that the "snow mixing ratio" dimension is not a physically-justified way to improve the results. However, it was never intended to build a fudge factor into the upgraded version of the forward model, but rather to use this as a straightforward way to investigate a number of interesting things: (i) it underpins Figure 9, which shows the stability of the results to potentially large errors in the modelled convective mixing ratio; (ii) it is also helpful in the situation-dependent parameter search (Table 6) and discussion (section 6.1). Here, the need to increase it in tropical convective areas to better fit the observations might indicate an error in the modelled convective mixing ratio, but it might also point to a need for broader convective cores, thicker anvils, or bigger and/or more scattering particles, as discussed in the text. Hence, the "snow mixing ratio" dimension is an important part of the work and I would like to keep it. However, its purpose could be introduced better in section 3.2, where I will try to add a few sentences in the revised manuscript.

Extensive changes are made at lines 217 - 236 to better introduce and explain the convective snow mixing ratio.

The situation-dependent results listed in Table 6 are interesting and make us think more about the physics in terms of how to select ice particles. Clearly, the "snow" particles in the tropics and higher latitudes are different – all the results seem to point out that tropical snow particles are denser than those in mid-latitudes. Or, maybe the "convective" and "large-scale" separation of clouds is not an ideal one after all. Microphysically, the anvil associated with tropical convections are distinctively different from the stratiform clouds associated with frontal large-scale uplifting. This may be an area of future improvement of the "best configuration". Adding some statements along this line in the conclusion section will be helpful.

This comment suggests that one way to improve the representation of convective anvils could be to treat them as a microphysically distinct cloud type, separate from the large-scale ice cloud generated by frontal uplift; hence one practical solution could be to treat anvil cloud as a separate hydrometeor type. This is a good suggestion and will be added to the conclusion of the revised manuscript.

This was added to the discussion on line 584-585; it did not fit perfectly in the conclusion.

A few other changes have been made, such as to use the version "13.0" for the relevant version of RTTOV-SCATT, which is more precise, and to make a few re-wordings to improve clarity, or fix small errors (for example on line 368)